

TECHNICAL REPORT 7808

THE HAZARD RANKING AND ALLOCATION METHODOLOGY:

EVALUATION OF THE WASTEWATERS FOR

CONTINUING RESEARCH EFFORTS

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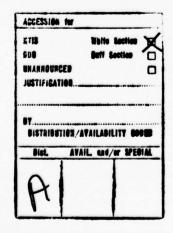
As part of this assessment, the Hazard Ranking and Allocation Methodology was performed on compounds of interest. This analysis is based on estimations of hazard and the quality of these estimates. The estimate quality is expressed as a numeric quantity called uncertainty. The most favored research project is that which will bring about the largest decrease in the product (hazard x uncertainty) per research dollar spent.

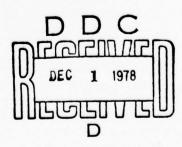
Data inputs to the methodology include pollutant discharges, populations (human and other species) at risk, characteristics of pollutant travel in streams (flow and travel time), effects of concern and their "cost," and toxicology data relevant to each effect for each compound. The data base was updated to reflect research findings. The procedures used are herein explained.

The systems analysis is performed in two parts. The first part is a hazard analysis. This gives a view of the compounds in a cost perspective and provides a means to weed out research projects which are very marginal in terms of allocation criteria. 2,4,6-Trinitrotoluene posed the greatest hazard of all compounds, although a large portion of this was from discharges not considered "condensate water." Other compounds which ranked high in hazard were 2,3,6-trinitrotoluene, 1,3-dinitrobenzene, and 5-amino-2,4-dinitrotoluene. The major component of hazard was to the environment (as expressed in terms of fish) rather than to humans (in terms of effects from ingestion of contaminated water).

The research allocation analysis was performed on 20 projects. They involved 10 compounds and two studies: (1) a lifetime mammalian study and (2) an in-depth acute aquatic bioassay. The analysis indicated that any compound/acute aquatic bioassay project was favored over any compound/mammalian project. The most promising of the former projects were for 2,4,6-trinitrotoluene, "condensate water" (considering the mixture as an entity), 2,4,6-trinitrotoluene, 1,3-dinitrobenzene and 4-amino-2,4-dinitrotoluene.

This was the first exercise of the methodology in support of munitions pollution criteria management. Thus, the stochastic characteristics of the methodology and how they impact upon results were reviewed in depth.





#### SUMMARY

This report documents the systems analysis of the Hazard Ranking and Allocation Methodology for compounds found in wastewaters from operations with 2,4,6-trinitrotoluene. The analysis was done in conjunction with a progress review of Contracts DAMD 17-75-C-5056 and DAMD 17-76-C-6060 with a major goal of planning further toxicological studies.

Prior to execution, a data base amenable to program algorithms had to be assembled. Demographic and hydrologic data had been previously defined. Discharge rates for compounds were, for the most part, based on analyses performed on "condensate water." Some "non-condensate water" discharge sources for 2,4,6-trinitrotoluene and 2,4-dinitrotoluene were identified. Environmental disappearance factors for the compounds were based on available vaporization and photolysis experimental information.

Dose-risk factors for fish effects were based on screening acute aquatic toxicity data from Contract DAMD 17-75-C-5056. Dose-risk factors for mutagenic potential in humans were based on the results of Ames/Salmonella mutagenic bioassays and scaled based on a long-term study of the tumorgenicity of 2,4-dinitrotoluene in rats. Dose-risk factors for chronic, non-carcinogenic effects in humans were either based on past experimental results (available for 2,4,6-trinitrotoluene, 2,4-dinitrotoluene, and 2,6-dinitrotoluene) or on default assumptions.

The hazard ranking was performed first. The algorithms presume all data are accurate, and provide an estimate of yearly adverse socioeconimic costs of the consequences of exposure to wastewater. Thirty specific compounds were analyzed, as was "condensate water" as a pseudocompound. The following hazards were obtained for the 10 highest-ranking compounds:

Compound	Hazard to Humans	Hazard to Fish	Total <u>Hazard</u>
2,4,6-Trinitrotoluene	694	2333	3027
"Condensate water"	1 69	2173	2342
2,3,6-Trinitrotoluene	12	766	778
2,4-Dinitrotoluene	184	332	516
1,3-Dinitrotoluene	86	410	496
5-Amino-2,4-dinitrotoluene	21	467	488
3,4-Dinitrotoluene	5	185	190
1,3,5-Trinitrobenzene	31	113	144
2,3-Dinitrotoluene	4	122	126
2,6-Dinitrotoluene	10	93	103

The main contribution to the 2,4,6-trinitrotoluene hazard is from sources not associated with "condensate water" discharges. On the basis of

condensate water alone, 2,4,6-trinitrotoluene would have ranked lower than 3,4-dinitrotoluene

These compounds were then processed to determine the predicted effectiveness of proposed research. This involves a stochastic analysis of the increase in confidence estimation that is expected to occur due to the research. Uncertainty factors are required for all elements of hazard data inputs. They are derived on an arbitrary or by concensus basis. The increase in confidence in hazard is represented mathematically by a decrease in the product of hazard x hazard's uncertainty as a result of the research. This decrease divided by research cost is a rational objective factor for the assessment of research. The economic argument for this is presented in the Appendix of the report.

Two projects were assessed for most of the highest-rated compounds above. The first was an in-depth aquatic toxicity test (AAT) at a cost of \$20,000 per compound. The second was an in-depth long-term mammalian feeding study (LTM) at a cost of \$400,000 per compound. The analysis indicates that any of the AAT-projects considered were expected to be more cost-effective than any of the LTM-projects. This was based on four replicate allocation runs, each with 100 stochastic simulations of scenario hazards. The more specific ranking is:

For AAT-projects: 2,4,6-trinitrotoluene

"condensate water"
2,3,6-trinitrotoluene
1,3-dinitrobenzene

5-amino-2,4-dinitrotoluene

2,4-dinitrotoluene 3,4-dinitrotoluene 2,3-dinitrotoluene 1,3,5-trinitrobenzene 2,6-dinitrotoluene

For LTM-projects: 2,4,6-trinitrotoluene

"condensate water" 1,3-dinitrobenzene

5-amino-2,4-dinitrotoluene

1,3,5-trinitrobenzene
2,3,6-trinitrotoluene
3,4-dinitrotoluene
2,6-dinitrotoluene
2,3-dinitrotoluene

The allocation procedures were studied in detail for characteristics of the analysis. Several that were noted were:

- a. The assumption of log-normal distribution was reasonable for hazards associated with toxicological study considerations. To some extent, the distribution depends upon the uncertainties assigned to input variables.
- b. The assumption of log-normal hazard distribution may become less reasonable for analyses of research projects other than toxicological studies. The allocation procedures may not be conceptually correct in such situations.
- c. Uncertainty contributions of important variables were capable of being identified.
- d. Because the objective factor for rating research projects involves operations on variables that are stochastically generated, it also has a stochastic nature.
- e. The amount of computer time required for allocation analysis will depend upon the criticality of the purpose of the analysis. For a rough analysis, one run with 100 to 300 simulations should suffice. If a more critical assessment is required, replicated runs are recommended. The procedure used in this study is believed to produce rankings which could be one or two positions out of place.

#### ERRATA

The values of S(FKL) and S(CFS) on line numbers 1291 and 1292, Figure 1, should read 2.2-2 and 6.7-2 liters/mg-year, respectively.

On page 40, the hazard of 2-amino-4,6-dinitrotoluene should be 5.

### TABLE OF CONTENTS

SUM	MARY	1.			•						•			•	•		•		•		•	•					•				•	1
INT	RO DI	JCT	101	1											•			•														9
TNT	WAS	STE	WAT	ΓER	S	•						•			•		•			•	•											9
	Pro Ind Mui	cor	poi	rat	ic	n	Wa	st	ev	vat	er	°S																				9 10 10
HRAI	M AS	5 A	PPI	IE	D	TO	) S	UF	RF#	A C E	. W	ΙΑΊ	EF	? F	POL	.Ll	JT!	10	١							•						12
THE	DA	ГА	BAS	SE														•											•			14
	Por Por Env Red Cor Eff	llu /ir ten nce fec	ticonr tic ntic ts	on men on rat an	Di Fa ic	s of	cha Di tor Do	sa sa se ses	pp (	Ra ea Con	te ra ·	es enc	e io	Ra	te Fa	e (	or to	ist	ar	its								 			• • • • • • • • • • • • • • • • • • • •	24 30 32 36 36 36 37
HAZ	ARD	AN	AL۱	/SI	S	A۱	ID	D I	S	CUS	SI	01	1															•				40
THE	ALL	.0C	AT.	ON	A	NA	LY	SI	S				•															•				46
	Res Sta All Obj	ati loc	state	i ca i on	l R	Co	ns ul	ic	le	ra t	ic I D	ns	CL	f	th	ne on	A1	10	) C a	ati •	or •		1e 1	tho •	odo •	10	93		•	•		46 47 50 56
CON	CLUS	510	NS	AN	D	RE	:C0	111	1E1	NDA	TI	01	IS															•	•	•		58
LIT	ERA"	TUR	Ε (	CIT	E	)				•																				•	•	63
APP	END:	X.	Α.	T	he	e E	co	nc	mi	i c	Ва	si	S	fo	r	HF	NAS	1			•				•		•					65
ACR	IYNC	MS	AN	o s	YN	1BC	ILS	U	SE	ED	IN	1 7	НІ	S	RE	PC	R														•	70
DIS	TRIE	BUT	IOI	V L	IS	Т																										72

### TABLES

1.	Compounds in "Condensate Water" and Their HRAM Mnemonic Codes .	11
2.	Line Numbers for Population Data, Flow Rates and Travel Times Used in Computations	24
3.	Compound Concentrations Used for "Condensate Water"	31
4.	Tests on Environmental Effects for TNT Wastewater Compounds and Selected Rate Constants	33
5.	Dose-Risk Slope Data Line Number Locations	38
6.	Hazard by Compound and Effect (Partial List)	42
7.	Risks Associated with Compounds for the Most Exposed Populations (Partial List)	44
8.	Hypothetical Data Base to Illustrate Sensitivity of Hazard to LMD	45
9.	Hazards from Table 8 Data Based on Different Values of LMD	46
10.	Comparison of Hazards: Deterministic vs. Stochastic	54
11.	Allocation Objective Factors Obtained after Selected Monte-Carlo Simulations	57
12.	Allocation Objective Factors and Estimate of 90 Percent Confidence Interval of Mean from Four 100 Monte-Carlo Simulation Runs	59
	FIGURES	
1.	Data Base for TNT Wastewater Analysis	15
2.	HRAM Representation of Populations at Risk from TNT Wastewaters of Joliet Army Ammunition Plant	25
3.	HRAM Representation of Populations at Risk from TNT Wastewaters of Radford Army Ammunition Plant	26
4.	HRAM Representation of Populations at Risk from TNT Wastewaters of Volunteer Army Ammunition Plant	27

5.	HRAM Representation of Populations at Risk from TNT Wastewaters	
	of Holston Army Ammunition Plant	28
6.	Roof-Top Test Data and Photolysis Reactor Time Estimates for	
	2,4-Dinitrotoluene	34
7.	Hazard Computations Corresponding to Equation (2)	41
8.	Research Projects for Allocation Evaluation	48
9.	Allocation Data from a 300 Monte-Carlo Simulation Run.	51

#### INTRODUCTION

The Hazard Ranking and Allocation Methodology (HRAM) was developed by SRI, International for Contract DAMD 17-75-C-5071. HRAM provides a framework which numerically represents the hazard that pollutants pose to human and non-human populations and a rational method for rating proposed research projects. The methodology is described in detail in the Contract Annual Report by Brown. The hazard computational portion of HRAM was operational at the US Army Medical Bioengineering Research and Development Laboratory in August 1976. The allocation methodology was added in December 1976. During 1977, improved algorithms were installed.

SRI, International is also performing research under Contracts DAMD 17-75-C-5056 and DAMD 17-76-C-6050. These studies involve wastewaters associated with 2,4,6-trinitrotoluene (TNT) production and munition loadings. The effort involves the identification of other compounds in such wastewaters; 29 such compounds were identified and their concentrations determined. Initial work was completed on the toxic and mutagenic properties of these compounds; an aquatic toxicity test and a microbial (Ames/Salmonella) mutagenic bioassay, respectively.

Given this number of compounds and the cost of possible additional toxicological studies, a meeting was held on 23-24 February 1978 to review research results from these contracts and plan future studies. As part of this assessment, a HRAM analysis was performed. This was the first full scale test of HRAM. This report documents the information which went into the analysis and the derived results. It also reviews aspects of the analysis that need to be considered in the interpretation of results, and aspects that need improvement.

#### TNT WASTEWATERS

Three general types of TNT wastewater are known: those from TNT production; those from incorporation of TNT with other explosives, primarily cyclotrimethylenetrinitramine (RDX); and those from loading of explosive formulations containing TNT into munitions. The HRAM analysis performed covered the first two types; for completeness, all three are discussed.

#### Production Wastewaters

TNT is produced by the stepwise nitration of toluene in the presence of sulfuric acid. The raw product contains about 96 percent TNT, 3 percent of other five trinitrotoluene isomers, at least two dinitrotoluene isomers, dinitrobenzene and trinitrobenzene.<sup>2</sup> The TNT isomers detract from the explosive and mechanical properties of TNT. They are largely removed by washing the molten raw product with "sellite," a basic

solution of sodium sulfite. The spent "sellite" has an intense red color (to the extent that it is almost black) and forms the major component of TNT wastewaters that has been considered for abatement from production. Other usual wastewater sources are: waters from scrubbers that collect fumes from the nitrators and TNT dust from bagging operations; routine washdowns of floors; washdowns of occasional spills; and some spent acid wastewater from initial washing of the raw product prior to the "sellite" wash.

TNT production at Volunteer, Radford, and Joliet Army Ammunitions Plants would involve discharges to surface waters.\* At present, none of these plants are in TNT production.

At Radford Army Ammunition Plant, the spent "sellite" is segregated from the other wastewaters and concentrated in open vats. The concentrate is sold to paper mills. The other wastewaters are subjected to settling and pH adjustment treatment prior to discharge.

At Volunteer and Joliet Army Ammunition Plants, all wastewaters are collected and concentrated in a partial evaporator. The more volatile compounds tend to distill into an aqueous solution called "condensate water." This water is discharged to surface streams, and is the TNT wastewater of concern at these plants. The concentrate is either sold to paper mills or incinerated. The compounds that have been identified and concentrations in "condensate water" analyzed are listed in Table 1.

#### Incorporation Wastewaters

Wastewaters from the incorporation of TNT with RDX are confined to Holston Army Ammunition Plant. In this process, the two explosives are added to a steam kettle, heated, and then transferred in molten form to a casting vessel. The molten mixture drips out of the vessel, solidifies, and is packaged. Wastewaters occur from the water floated from the molten mixture (the RDX is slightly moist when added to TNT), washdowns, and fume scrubbers.

#### Munition Loadings Wastewaters

These wastewaters arise from washdown of floors and from steam-out of rejected fills. These wastewaters, where discharged to surface waters, are first treated with activated charcoal, which greatly reduces TNT concentration. Where not so treated, wastewaters are stored in open sumps or ponds where evaporation or percolation can occur. In either case, the volumes of wastewaters involved are not large compared to production

<sup>\*</sup> Newport Army Ammunition Plant also has a TNT production facility. However, total incineration of all TNT wastewaters is expected to be performed.

TABLE 1. COMPOUNDS IN "CONDENSATE WATER" AND THEIR HRAM MNEMONIC CODES

Compound	Code
2,4,6-Trinitrotoluene	TNT
2,3,6-Trinitrotoluene	T11
Toluene	TOL
2-Nitrotoluene	2NT
4-Nitrotoluene	4NT
2,3-Dinitrotoluene	23D
2,4-Dinitrotoluene	- 24D
2,5-Dinitrotoluene	25D
2,6-Dinitrotoluene	26D
3,4-Dinitrotoluene	3 4D
3,5-Dinitrotoluene	3 5D
1,3-Dinitrobenzene	DNB
3,5-Dinitroaniline	DNA
3-Methy1-2-nitrophenol	3DP
5-Methy1-2-nitropheno!	5DP
3-Nitrobenzonitrile	3NB
4-Nitrobenzonitrile	4NB
2-Amino-4-nitrotoluene	AN6
2-Amino-6-nitrotoluene	AN8
3-Amino-4-nitrotoluene	AN7
1,3,5-Trinitrobenzene	TNB
2-Amino-3,6-dinitrotoluene	ADB
2-Amino-4,6-dinitrotoluene	2AD
3-Amino-2,4-dinitrotoluene	AD9
3-Amino-2,6-dinitrotoluene	BAD
4-Amino-2,6-dinitrotoluene	4AD
4-Amino-3,5-dinitrotoluene	ADC
5-Amino-2,4-dinitrotoluene	ABD
2,4-Dinitro-5-methylphenol	DNP
1,5-Dimethy 1-2,4-dinitrobenzene	DDB
"Condensate Water" (Composite)	TCP

wastewaters. Moreover, since product TNT is used in this operation, many compounds that are in "condensate water" would not be expected in these discharged wastewaters. Finally, HRAM algorithms have not been developed to handle the pond-storage situation.

#### HRAM AS APPLIED TO SURFACE WATER POLLUTION

A brief review of the methodology is presented to explain data inputs and processing. For more detail, either reference 1 or 3 should be consulted. HRAM data inputs are based on available hard data, reasonable estimates, or default values. Quite often, inputs must be transformed for use in HRAM. Where pertinent to the discussion, these transformations will be reviewed. Otherwise, reference 3 should be consulted.

Populations considered subject to pollutants are defined (N).<sup>††</sup> For humans (HUM), these are communities which draw drinking water supplies from the surface water containing the pollutant. For fish (FSH), these are some representation of the fish population expected in a reach of the surface water. For each population group, a representative flow rate of the surface water (SMF) and a travel time for the pollutant to pass from its point of entry to surface water to the population (SMT) is specified. For fish, this is generally taken at the spatial mid-point of the population group.

For each compound, a mass loading rate of the pollutant to surface water (Q) is defined. A water treatment retention factor (R) is also defined, which accounts for raw water treatment procedures in waterworks. An environmental disappearance factor (LMD) is defined, which presupposes that a first-order decay of the pollutant with travel time occurs. Then, for each population group involved, a pollutant concentration is computed:

$$C = (1/SMF) *Q * R * exp(-LMD*SMF)$$
 (1)

For each compound, adverse effects of concern are defined. Each effect is assigned a socioeconomic cost (V). A linear relation is presumed to apply between the dose of a compound and the probability that an adverse effect will occur in a year to an "average" individual in a population. The slope of this dose-risk relation (S) is used in HRAM. HRAM allows for use of a threshold; however, practice has been to assume no threshold. For effects considered of a chronic nature in humans, a concentration-dose conversion factor (SMB) is applied. HRAM provides a SMB of 1.0 if this factor is not specified. This allows for processing of S in terms of concentration for fish populations.

However, some could occur in environmental processes that TNT undergoes. See Pollution Discharge Rates, page 30.
 The notations that appear are used in HRAM.

The yearly hazard of a given compound, for a given effect, and to a given population group<sup>+</sup> is computed:

$$H = C * SMB * S * V * N$$
 (2)

Equation (2) can be summed to provide less restricted hazards, such as:

Hazard (one effect and compound) = 
$$\Sigma$$
 H (3)  
Populations

and

Hazard (one compound) = 
$$\Sigma$$
  $\Sigma$  H (4)  
Effects Populations

Equation (2) would be accurate, within the scope of the assumptions, if the variables were well known, which is not usually the case. The allocation concept is based on this. An uncertainty is associated with each variable. The uncertainty numerically represents the existing state of knowledge about the variable. Reference 3 largely deals with current practices in the assignment of uncertainties.

For allocation purposes, the variables are processed as probability distributions, to quantitatively account for their inaccuracy. Three options exist for the type of distribution, and with each option, a definition of uncertainty in terms of probability concepts. If V is any variable,  $\overline{V}$  its estimated mean [the value used in Equation (1) or (2)] and U its uncertainty, the options are:

- 1. Additive -- V is normally distributed with estimated mean  $\overline{V}$  and standard deviation U/2. U has the format " + nn."
- 2. Percentage --  $V/\bar{V}$  is normally distributed with estimated mean of 1.0 and standard deviation U/200. U has the format " + nn P."
- 3. Log-normal -- Log V is normally distributed with estimated mean Log  $\overline{V}$  and standard deviation Log  $\overline{V}$ . U has the format " \* nn."

Hazard is also some form of probability distribution and has an uncertainty. The statistical inference given to hazard and its uncertainty, stated for a log-normal distribution, is: let  $\overline{\text{H}}$  be the value of uncertainty computed by either Equations (2), (3) or (4). Let " \* U<sub>H</sub> " be its uncertainty. Then, if h is any random selection from the distribution,

<sup>&</sup>lt;sup>†</sup> Strictly speaking, hazard is qualified by six subscripts. This explanation has been restricted to surface water. Moreover, each population group is in terms of a location, a type of population (human or fish, for example) and a numerical index.

### Probability $(H/U_{H} \le h \le HU_{H}) \stackrel{\sim}{=} 0.95$

(5)

The 95 percent range that is associated with hazard and its uncertainty is central to the allocation methodology. Research is considered a process which improves upon the accuracy of one or more variables. This can be expressed as a reduction in the variable uncertainty to a defined numerical value. This is reflected in a reduction in the range of hazard as stated in Equation (5). This reduction was shown in reference 1 to represent a benefit. This benefit divided by research cost provides a ratio which can be used as an objective factor to compare different research projects. Appendix A reviews the economic argument behind this concept.

Deterministically, the uncertainty of hazard is not readily computed. Stochastically, it is computable if the hazard distribution is specified in advance. HRAM assumes this distribution is log-normal. Monte-Carlo simulation techniques can then be used. Several iterations are required; in each iteration, Equation (2) is evaluated based on random selections of variable values according to their distributions. Then, if required, summations to Equations (3) or (4) are performed. After the second iteration, the log-normal mean and uncertainty of hazard can be back-calculated. This process is performed twice per iteration, once for the current situation, once for the post-research situation. The hazard ranges for the current and post-research situations are then computed and the ratio determined.

#### THE DATA BASE

The data required to compute hazard for the TNT wastewater situation appears in Figure 1. Each line, which is a data entry, has an identification number on the right hand side (Line ID.). Line numbers will be cited. All variables have subscripts; the subscripts are defined first. The subscript for surface water transport, H2O, is pre-defined. Subscripts are in the form of three-character mnemonic codes. The subscripts corresponding to locations occur on lines 30 - 51. The subscripts corresponding to compounds occur on lines 80 - 400. The subscripts corresponding to effects occur on lines 450 - 470. The subscripts corresponding to population types occur on lines 490 - 500. Numerical subscripts are used to define specific population groups.

Data documentation is included in two notebooks.<sup>4,5</sup> These notebooks include the background and computations employed to develop the data. Where other references are not herein cited, these notebooks are the data sources.

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CHE230 CHE230 CHE350 CHE350 CHE360 CHE360 CHE360 CHE360 CHE360 CHE360 CHE360 CHE360 CHE360			23-DNT 34-DNT 34-DNT 35-DNT 236-TNT 236-TNT 248-TNT 248-TNT 248-TNT 342-ENT 342-ENT 342-ENT 342-ENT 342-ENT 343-ENT 34	000000084 000000088 000000088 000000088 000000088 000000	02/14/18 02/14/18 02/14/19 02/14/19 02/14/19 02/14/19 02/14/19 02/14/19 04/10/19	8
CHECON CH			JOURNAY INCOMENTAL INC	00000101 00000101 00000101 00000102 00000103 000000100 0000000100 000000100 000000100 000000	02/14/18 02/14/18 02/14/18 02/14/18 01/04/17 01/04/17 04/10/18 04/10/18 04/10/18	36 5 7 7 7 7 9 7 9 9 7 9 9 9 9 9 9 9 9 9 9

LISTING OF MODULE TSTIB

SURFACE WATER CATA BASE

54TE 64710/78 TIME 0950

RUN NC. 6165 DESCRIPTION

Figure 1. Data Base for TNT Wastewater Analysis.

	AUN NO. 6165	3116	C4/10/78 TIME 3951	LISTING OF MCDULE TSTIB	15118	
1,000   1,00	EFFFKL			FISH KILL	030000410	
### ### ### ### ### ### ### ### ### ##	*TPHU*			FUMAN	C0CC0490	
Control   Cont	25.54			<b>u</b> ,	0050000	
Main			13 0000		0000051	04/26/11
Control   Cont					6190000	11/01/20
REDIFFEST TO STATE TO THE PROPERTY COUNTY OF		. ~			7190000	05/10/77
VCLMCCCHW 1 100000 CT * 1.1 TST RMZLS C000053 VCLMCCSH 2 3.99 JF 2.3 TST RMZLS C0000614 VCLMCCSH 3 3.99 JF 2.3 TST RMZLS C0000617 VCLMCCSH 4 2.3 TST RMZLS C0000617 VCLMCCSH 5 2.3 TST RMZLS C0000617 VCLMCCSH 6 2.3 TST RMZLS C0000617 VCLMCCSH 7 3.29 JF 2.3 TST RMZLS C0000617 VCLMCCSH 6 2.3 TST RMZLS C0000617 VCLMCCSH 7 1.3 FF 2.3 TST RMZL 17 C0000617 VCLMCCSH 7 1.3 FF 2.3 TST RMZL 17 C0000617 VCLMCCSH 7 2 TST RMZL 17 VMZL 17 VMZ		,		TST	000000	05/10/17
VCLHCESH 2 3-9+3 CT 4 1.1 ISTRIBAZIS C0000651 VCLHCESH 2 3-4+4 F 2.1 ISTRIBAZIS C0000651 VCLHCESH 3 5-3+5 F 2.3 ISTRIBAZIS C0000651 VCLHCESH 4 22-3+5 F 2.3 ISTRIBAZIS C0000671 VCLHCESH 5 3-3+4 F 2.3 ISTRIBAZIS C0000671 VCLHCESH 6 32-3+5 F 2.3 ISTRIBAZIS C0000671 VCLHCESH 7 32-3+5 F 2.3 ISTRIBAZIS C0000671 VCLHCESH 1 10-10-10-10-10-10-10-10-10-10-10-10-10-1		_		TS11	00000030	04/26/17
VOLHACESH 2 3.949 PF 5.23 TSTIRMSZLY GODOJO72 VOLHACESH 2 3.949 PF 5.23 TSTIRMSZLY GODOJO73 VOLHACESH 3 5.949 PF 5.23 TSTIRMSZLY GODOJO73 VOLHACESH 3 5.945 PF 5.23 TSTIRMSZLY GODOJO73 VOLHACESH 4 5.945 PF 5.23 TSTIRMSZLY GODOJO73 VOLHACESH 4 19.945 PF 5.23 TSTIRMSZLY GODOJO73 VOLHACESH 4 19.945 PF 5.23 TSTIRMSZLY GODOJO73 VOLHACESH 4 19.945 PF 5.23 TSTIRMSZLY GODOJO73 PF 6.23 TSTIRMSZLY GODOJO74 PF 6.23 TSTIRMSZLY GODO		7		TST	(6000631	04/26/17
VULHECESH 2 3.349 #F 6.24 ISTIGNEZIS COCCOLOR VULHECESH 3 5.046 #F 6.24 ISTIGNEZIS COCCOLOR VULHECESH 4 2.046 #F 6.24 ISTIGNEZIS COCCOLOR VULHECESH 4 2.046 #F 6.24 ISTIGNEZIS COCCOLOR VULHECESH 4 2.046 #F 6.24 ISTIGNEZIS COCCOLOR VULHECESH 4 2.040 **		-			000000011	11/01/50
VOLHACESH 3 5.3-5 5 F 5.3 ISTIBARIIS COUNDOY 3 VOLHACESH 4 5.3-5 5 F 5.3 ISTIBARIIS COUNDOY 3 HCLACCHUM 2 1,34-5 C 7 1,34-5 C 7 HCLACCHUM 3 1,34-5 C 7 2,3 ISTIBARII COUNDOY 3 HCLACCHUM 4 1,34-5 C 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 2 1,34-5 C 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 3 1,34-5 C 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 4 1,34-5 C 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 5 1,34-5 C 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 5 1,34-5 C 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 6 1,3-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,4-6 F 7 2,3 ISTIBARII COUNDON 7 HCLACCHUM 1 3,4-6 F 7 2,4-6 F 7 2,4-6 F 7 2,4-6 F 7 HCLACCHUM 1 4,4-6 F 7 2,4-6 F 7 2,4-6 F 7 HCLACCHUM 1 4,4-6 F 7 2,4-6 F 7 2,4-6 F 7 HCLACCHUM 1 4,4-6 F 7 2,4-6 F 7 2,4-6 F 7 HCLACCHUM 1 4,4-6 F 7 2,4-6 F 7 2,4-6 F 7 HCLACCHUM 1 4,4-6		7			CCCCC6 12	05/10/17
CHARTER         1.3 ISTIBAZIO         CO000674           CHARTER         2.3 ISTIBAZIO         CO000674           CHARTER         1.0 PCRRISTON         CO000674           CHARTER         1.0 PCRRISTON         CO000674           CHARTER         1.0 PCRRISTON         CO000770           CHARTER         2.1 STIBAZII         CO000801           CHARTER         2.3 ISTIBAZII         CO0000003           CHARTER         2.3 ISTIBAZII         CO0000003           CHARTER         2.3 ISTIBAZII         CO0000003           CHARTER         2.3 ISTIBAZII         CO000003           CHARTER         2.3 ISTIBAZII         CO00003           CHARTER         2.3 ISTIBAZII         CO00003           CHARTER         2.3 ISTIBAZII         CO00003           CHAR		3		* 2.3 TSTIB#2/15	00000003	11/01/50
1		4		* 2.3 TSTIB#2/15	(0000674	C5/10/17
1,49.5   1		_			0000000	01/25/17
1 1985 CT		~		E/NE KNOX	00101760	09/28/16
\$4		~		+ 20P KNOXVILLE	000000	02/58/16
\$4 1 371842/17 CCCCC800  \$54 2 37143 5F		•			08/20000	04/26/11
55.4 2 571143 5F		_			0080000	05/10/17
54 1		7			C0c00301	05/10/17
554 1 1.19 6 15		~ .			CCC00802	05/10/11
1.14-6 15 2		_			50000830	01/11/11
34 5 1746 5F	JULI ZEFSH		. 1+6		(63)3831	22/10/150
3.44 bb / CT	JULIA ZUE SH	7 .			00000832	05/10/10
1.0 15 75	JULHELY 3H	•	4 .		00000833	11/01/50
3+5 15 7CT * 1.01 CANCER COUNCESSES 5.0 LT / YR * 1.01 COUNCESSES 5.0 LT /	SHORE		A .	AL ACOL	18800000	01/03/17
3+5 55 7CT * 1.01 CANCER COUNTY STATE	STORING TO			OT VINE	2880000	71/03/11
1.0   \$6   \frac{4}{4}  \	HUMC			CANCER	C0000884	01/03/17
500 LT /YR	FSHFKI		\$ 9		58833003	77/20/10
500 LT /YR	48240 F2CC				0450000	01/11/10
500 LT /YR       * 1.01       C0C00553         500 LT /YR       * 1.01       CCC00954         500 LT /YR       * 1.01       CCC00955         500 LT /YR       * 1.01       CC000956         500 LT /YR       * 1.01       C0000957         500 LT /YR       * 1.01       C0000957         500 LT /YR       * 1.01       C0000956         500 LT /YR       * 1.01       C0000956         500 LT /YR       * 1.01       C0000966         500 LT /YR       * 1.01       C0000966         500 LT /YR       * 1.01       C0000966         500 LT /YR       * 1.01       C0000967         500 LT /YR       * 1.01       C000097         500 LT /YR	MATCL HZCC		-	* 1.01	03000551	02/16/78
500 LT /YR	482NT F2CC		-	* 1.01	C3033952	92/16/78
500 LT /YR	184NTH2CC		5	* 1.01	66600000	02/16/18
500 LT /YR	48230F2CC		_	* 1.01	CCC00954	02/16/76
500 LT / YR	48.250 H 20.0		_ !	1.01	60011955	02/16/78
500 LT /YR	48340F2CC		5	1001 *	00000000	02/16/78
500 LT /YR	48350F2CC		_ :	1.01	2500000	02/16/18
500 LT /YR	2041116			10.1	8550000	02/10/18
500 LT /YR	MRAN8H2CC			1:01	00000000	02/16/78
500 LT /YR	MBANTHOCC		5	1.01	19600000	02/16/78
555 LT /YR	MBACBF2CC		1	10.1	00000962	02/16/78
500 LT /YR	48 4 09 H 2 C C		٦	* 1.31	00000963	C2/16/1E
500 LT /YR	48BADH 2CC		17	* 1.01	00000000	02/16/78
500 LT /YR	#BACCH2CC		5	+ 1.01	00000000	02/16/78
500 LT /YR	46EBDF2CC		1	10.1 *	99507000	02/16/78
5JJ LT /YR	MRTNBHZCC		-	* 1.01	29600000	02/16/78
500 LT /YR	MRDNBF2CC		-	10.1 *	53653568	02/16/78
500 LT /YR * 1.01 CCC00970 500 LT /YR * 1.01 CCC0C5.71 500 LT /YR * 1.01 C0000972 500 LT /YR * 1.01	430CBH2CC		5	10.1 +	69500000	02/16/78
5.) LT /YR	MBONAHZCC		ב'	10.1 *	02600000	02/16/76
500 LT /YR * 1.01 60000972 500 LT /YR * 1.01 60600973	483CPH2CC		_	10.1	00000571	02/16/78
500 LT /VR * 1.01 CUCC0573	MB 50PH 2CC		-	* 1.01	00000972	02/16/70
	M84NDF2CC		5	1.01	CU00005	32/16/78

	02/16/78	02/16/78	11/11/10	01/11/10	11/11/10	11/04/11	11/04/11	11/04/11	02/16/18	71/11/10	81/91/20	11/01/11	71/11/10	11/13/11	01/11/17	02/16/78	11/10/77	11/17/11	11/11/10	11/10/11	01/12/11	11/13/11	77/11/17	77/31/20	1000	87 /91 /70	02/16/78	32/16/18	02/16/78	02/16/78	02/16/76	02/16/18	11/22/11	01/14/11	01/14/17	11/22/11	01/14/17	11/14/17	BL141140	01/12/130	21/1//20	81 (81 /26		05/16/18			92/16/78	02/16/78	02/16/76	~			02/16/18	•	02/16/78	02/16/18	02/10/78	02/16/78	
15718	\$2 500000	00000075	C850C000	06600000	00001020	06331363	00001061	00001062	00001180	06110000	C000120J	00001203	00001204	00001505	00001206	76216000	00001000	0621000	16710000	00001252	00001253	0 100 1254	00001255	10000	00000	0001280	00001281	00001282	06710000	16210000	00001292	00001320	00001321	00001322	00001323	00001324	00001326	00001327	00001330	000000000000000000000000000000000000000	20000	260000	00001333	00001334	00001335	00001336	00001337	00001338	00001339	33031341	245	24670000	64610000	COCO 1344	00001345	30031346	00001347	00001348	
LISTING OF MCDULE						STANCARD	STANCARD	STANCARD	CNT-SCALED		TST18#2/39	TST18#2/37	TST18#22 DEF	ST18#2/37		15TIB#2/39	TCT 18#3/64	04 /7#91 16		18#2/31	SRI 96LC50 DATA	TSTIB#2/46		TCTIBA37 DECLT	TALL CONTROL	OF SCALED	LCSO SCALE	TO EXTRAP	CNT-SCALED	LC50 SCALE	STD EXTRAP	DNT-SCALED	STIB#2/58	ST18#35		TST 18#2/58	TST18#2/57	TST18#2/57					-					STD EXTRAP	STO EXTRAP									STO EXTRAP	
713	10.1	1.01	1.01	1.01	1.01					10.1 *		* 33 T	1 10.1 +		10.1 *	0.00			10.1		\$ 0.5	1 01 +									* 15 \$	* 20 0	1 ~	1 7 *	10.1 *	* 71	1 101 1											* 15 8	* 15 5									* 15	
0360	æ.	YR	YR	YR	YR	Y.	YR	YR		YR	MG YR		YR		YR	MG YR			×		MG YR		Y.B.	0 > 0 7	•		MG YR				MG YR			MG YR	YR		YR	MG YR								MG YR		MG YR	MG YR	MG YR					MG YR		MG YR	_	
TIME	Sub LT AVR	5	5	-	5		5		5.4-4/GM	500 LT /YR	LT /MG	W5.	500 LT /YR	4.5-5/GM	500 LT /YR	1 / MG			200 LI /YK		3.3-3 LT /MG YR	2-4/6M	500 LT /YR	V (M)		2010	2 LT /MG	) MC		LT /MG	6.7-1 LT /MG YR	7-5/GM	4.5-6/GM	5.0-3 LT /MG YR	500 LT /YR	1.1-4/GM	500 LT /YR	LT /MG	4-2 IT /MG	7 / 1	7 / 10	2	1 / MG	9 L .	LT /MG	-2 LT /MG	) MG			LT /MG	I / MC	2000	DE/ 17.	) H / H ?	LT /MG	LT /MG	•	LT /MG Y	
04/10/78 TIME	-	, 5	5	-	5	1	5			5	LT /MG	5-4/GM	500 LT	4.5-5/GM	1	1 / MG	2				-3 LT /MG	14-	-	V 11 /NC V		2010	S LT /MG	) MC		LT /MG	LT /46	7-5/GM	4.5-6/GM	/ MG		1.1-4/GM		5-2 LT /MG	I / MC	7 / 1	7 / 10	2	0 L L	9 L .	LT /MG	LT /MG	.5 LT /MG	DW/ L7	LT /MG	LT /MG	I / MC	2000	DE/ 17.	7 / 10	LT /MG	LT /MG	LT /MG Y	LT /MG Y	
TIME	-	, 5	5	-	5	1	5	500 LT		5	LT /MG	4.5-4/GM	500 LT	INTH2CCTG 4.5-5/6M	1	11 11 1MG		E0/6-8	17 005	3-6/6	-3 LT /MG	14-	11 005	1 0-7 1 7 / WC ×	HO75-7 L	E9/C-+-/	1.9-2 LT /MG	) MC	2.2-4/GM	2.2-1 LT /MG	LT /46		260H2CCTG 4.5-6/GM	/ MG		26DH2CCTR 1.1-4/GM	500 LT	1.5-2 LT /MG	2-4-2 IT /MC	7 0-3 17 /MG	2 K 2 C 2 K	DH/ 17 3-C-7	1-0-1 LI / MG	2.3-1 LT /MG	2.3-1 LT /MG	1.4-2 LT /MG	.5 LT /MG	DW/ L7	LT /MG	5.2-2 LT /MG	3.8-1 17 /86	2 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	3.1-2 LI /MG	0.4-2 LI /MG	S 2.3-2 LT /MG	1.2-1 LT /MG	2.9-1 LT /MG Y	4.0-2 LT /MG Y	

	02/16/78	02/16/78	02/16/18	02/16/78	02/16/78	02/16/78	02/16/78	11/04/11	11/04/11	11/04/11	03/30/76	03/30/78	02/30/16	03/30/78	03/30/78	03/30/78	03/32/78	01/05/50	03/30/78	03/30/78	03/30/18	03/30/76	03/33/78	03/30/78	03/30/78	03/30/18	03/33/18	03/30/18	03/30/78	93/30/18	03/03/18	03/03/16	03/03/18	32/16/18	02/16/78	02/16/78	02/16/78	92/16/78	02/16/78	02/16/78	32/16/78	02/16/78	02/16/78	02/16/18	02/16/78
15718	33031349	00001350	00001352	00001353	00001354	00001355	00001360	00001362	00001364	00001365	99610000	00001367	00001300	00001370	00001371	00001372	90031373	00001375	00001376	11610000	00001378	00001379	60001381	00001382	00001383	00001385	00001386	00001347	00001388	00001389	00001461	00001462	00001463	59510000	00001465	00001467	00001468	00001469	00001410	00001471	00001472	00001473	00001474	00001415	00001476
LISTING OF MODULE TSTIB	STO	15 STO EXTRAP	510	STO	STO		25 WEIGHIED DEINI		-	3		4 LC50 SCALE					4 LC50 SCALE					4 LCSO SCALE				4 LCSU SCALE				4 LCSU SCALE	10			20 DAI - SCALED	20 CNI-SCALED		20 ONT-SCALED								20 CNT-SCALED
	~	* *	· *	*	*	<b>*</b>	* *	•	* ~	YR *	*	* *	٠.	. ~	*	<b>*</b>	<b>* *</b>		* ~	œ	*	* *	*	*	* *	× ×	ΥR	* * *	* *	* *	. *	*	•	•	• •	•	•	•	•	•	•	•	•	•	*
04/10/78 TIME 0550	2 LT /MG	2.0-2 LT /MG Y	2 LT /MG	2 LT /MG	3 LT /MG	/#G	1-4/6×	5-5/6M	) M G		3 LT /MG	2.6-3 LT /MG Y	- L	2 LT /MG	LT /MG	LT /MG	8.3-1 LT /MG Y	3 - 1 / WG	LT /MG	LT /MG	LT /MG	2-1-2 LT /MG Y	LT /MG	LT /MG	LT /MG	6-8-3 LT /MG Y	LT /MG	LT /MG	LT /MG	3 1-3 17 /46 4	10 M	1.5-6/GM	6.0-6/GM	F9/4-4-1	8-0-5/GM	1.5-4/GM	5.6-5/GM	3.7-5/GM	1.4-4/GM	4.5-4/GM	7.8-5/GM	8.4-5/GM	4.9-5/GM	8.7-5/GM	1.1-3/6M
DATE	CCBH2CCFS	CNAH2CCFS	50PH2CCFS	4NDH2CCFS	FS	DNPH2CCFS	CPHZCC	CPH2CCTR	TCPH2CFKL	CPH2CCFS	CLHZCFKL	2NT H2CFKL	30H2CFK1	SOHZCFKL	40H2CFKL	SOHZCFKL	11H2CFKL	ANSHZEKI	ANTHZCFKL	CBH2CFKL	C9H2CFKL	ADH 2C FKL	BDHZCFKL	N3H2CFKL	DABHZCFKL	DNAHZCFKL	3CPH2CFKL	SCPH2CFKL	4NDH2CFKL	SAUHZUFKL	CL H2CC	ZNTH2CC	4NT H2CC	235H2CC	40H2CC	350H2CC	N6H2CC	ANBHZCC	AN7H2CC	ACBH2CC	AC9H2CC	BADH2CC	OCH2CC	230H2CC	TABH2CC

	02/16/78	02/16/78	3/11/18	03/03/10	81750750	81 181 170	81/91/70	81 /81 /20	92/100/18	02/08/18	1/00/6	03/08/18	03/08/18	11/52/11	11/67/10	01/00/10	01/00/10	03/00/10	01/00/50	03/08/18	03/08/78	03/08/78	03/08/18	03/08/78	03/08/78	02/16/18	03/38/18	03/08/18	03/17/18	03/08/18	03/08/18	03/08/18	03/08/18	03/08/18	02/08/18	87 /80/50	03/08/78	03/08/78	03/08/18	03/08/18	03/08/18	03/08/18	03/08/78	03/08/18	03/08/78	03/08/18	03/08/18	03/08/18	03/08/18	82/80/50	81/89/50	95/16/78	03/08/18
TSTIE	00001478	00001479	60331483	10000	18410000	7841000	58410000	1811000	68410000	06/10000	15,10000	0001000	19/10000	00010000	00001810	00001820	00001037	00001832	2610000	00001835	00001836	00001837	00001838	00001839	00001840	00001841	00001842	00001843	00001844	00001845	00001846	00001847	00001848	00001849	00001000	16810000	30031853	00001854	00001855	00001656	00001857	00001858	65810000	00001860	00001661	00001862	00031863	00001864	00001865	33331866	00001867	00001868	69810000
LISTING OF MODULE	* 20 ENT-SCALED	* 20 DNT-SCALED							1 2 1	100	00/2#81181 0 6 +	13.	75/18#5/20	12	87#81 ISI 18# #		1 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	444	4 4 4 4		VAAP	VAAP	VAAP				* S VAAP SAMPLES	* 5 VAAP SAMPLES				VAAP	VAAP	* 5 VAAP SAMPLES	A A A A		VAAP	VAAP		VAAP	VAAP	AAA	VAAP	VAAP				VAAP			* / VAAP EXIKAP		* CAAP EXTRAP
CATE 04/10/78 TIME 0950	*:/ S - 8 - 5	1.8-3/6M	N. 1 - 5 - 1	H9/9-5-1	1.3-0.6H	5.4-5/CH	1.7-3/6	3.3-2/6#	25		2 5	2	S C	2	4.9+3 KG / YK	2 5	9 4		2 3	N C	× ×	×	¥	Y C	8		25 KG /YR	1.5 KG /YR		¥	9	YC.	S .	8X/ 9X 011		2 2	5 X C	9	.5 KG /YR	1.5 KG /YR	9	y S	×	¥C	9	×	y Y	S X	×	9 9	×		25 KG /YP
54N NO. 6165	S OFBHOLD							5	.,,		- (		7	2	C ZADYALHZO	ν,		7 -	- ^		^	, 0	۰ ۳		-	<b>«</b> 1	7	Q ANTVOLHED	G ACBUCLHZD	4	T	4	4	O TNBVCLH23	20	DONALLES O		-	Q 4NDVCLHZG		C	Q 4ADJCLHZC	2			Q 4NTJCLHZS	2	7	3			C ANGJELP29	C ANSJETH 3C

	03/08/18	93/11/18	03/08/16	03/09/18	03/38/78	03/08/18	03/08/18	03/08/18	03/08/78	03/08/18	03/68/78	03/08/18	03/08/78	03/08/18	11/25/11	03/03/78	91/01/60	09/10/76	92/10/16	04/26/11	01/15/11	01/12/17	01/12/11	01/12/11	12/13/76	12/13/76	12/13/16	12/13/16	09/13/76	92/10/16	71/21/10	71/97/10	02/14/19	05/14/16	39/14/76	92/14/16	10/02/16	10/65/76	10/05/76	10/05/16	91/77/71	1777771	04/26/17	04/26/11	92/15/16	05/15/76
15716	00001870	00001871	00001872	00001973	00001874	00001875	00001877	91910000	36331879	00001881	60301882	00001843	00001884	000000000	00002050	0000000	00002000	00005000	00002100	00002120	00005170	00002171	00002112	00002173	00002230	00002231	00002232	00002233	00002200	00002280	00002290	00002300	00002350	00002360	00032370	CCC02383	00005400	00005401	00005405	00002403	00002430	00002451	00002480	0900000	00002530	39092549
LISTING OF MODULE	VAAP EXTRAP					VAAD EXTEAD			VAAP EXTRAP					VAAP SAMPLES		TST18#2/38	TST18P#121	TST 18P#121	ST 18P#121	ST 18#2/111	ST 18#135	ST 18#135	15118#135	15718#135	ST 18#135	TST 18#135	TST18#135	15118#135	1.4 TST 18P#121	ST18P#121	TST18P#121	TST18#2/114					15118#131-132	TST 18#131-132	5118#131-132	5118#131-132	2 0	2 0	STIB#2/114	STI8#2/114	TST18#128	1ST18#128
711	× 1 *						*		* +					* *					1.5	1.90	1 1.5 1							1.1 +	1 4-1 *	1.5 1		10.2 *		* 1.5	* 1.5				- '			* 1.7				* 3.0 1
C+/10/78 TIME 0950	1.5 KG /YR	6	×	S.	90 KG /YR		× 6	Š	55 KG /YR	2 2	×	Š		690 KG / KR	200	¥6	70		2.81.07					8.31 DY	5	-	ב'	1.32+12 LT /YR	2.85+12 LT /YR	5		20 0.14								¥3 C.88	20 80.			L u	-	1.38+11 LT /Y?
-																																														

40N VO. 6165 DA	DATE	04/10/78 TIME 0950	LISTING OF MCDULE	TSTIE	
		3.02+12 LT /YP		00002550	05/15/16
SMFVOLFSF 4		5	-	00002560	05/15/16
		5		0037583	10/05/76
		-		00002581	10/05/76
			* 1.05 TSTIB#130-131	00032542	10/05/76
		5	* 1.1 TSTIB#2/115	00002583	04/26/11
SMFHOLFSF		-	* 2.0 TSTIB#137	00002630	12/22/26
		-	* 1.2 TSTIB#137	00002631	12/22/16
		5.65+11 LT /YR	57 18#137	00002632	12/22/16
LMOTATH2C		71/YR		00302660	03/08/18
L40240H2C		25/YR		JU07268U	03/68/78
LMD440H2C		77/YR	+ 41P VOLIPHCTI	00002681	33/38/78
LMD2AJH2C		20/YR		CCC02632	03/08/78
LMD260H2C		94/48		00002120	03/68/78
LMJTCPH2C		38/YR		00002740	03/08/78
LMDTCLH2C		660/YR		00002811	03/08/78
LMD2NTF2C		126/48		02012812	J3/68/18
LMD4NTH2C		185/48		00002813	03/08/18
L40230H2C		27/148		00002414	03/08/18
C*0.250H2C		17//43		00002815	33/08/18
LMC340H2C		12/78		00002816	03/09/18
LACSPONSE		IVYR		00002417	33/63/18
LMJT11H2C		71/7	7.75	00002818	03/68/78
LACANGHAL		23/62	V J L Z	00002819	03/68/18
LMCANGHZC		20/73	V:)L 2	69332823	13/63/18
LMCANHAL		16/48	7.76	00002821	03/08/78
LYCAURHAL		22.07	VJL2	00002822	03/08/18
LACABARA		22/11	V 36.1	33032423	03/68/78
LACEADHZL		23720	1707	90905854	03/68/18
LMCACHAC MAY BOLD		8 175 T	11044 1104 455	00002825	03/58/18
L CABOLIZA		82/51	V 21.2	00002827	46/00/60
L WOONBHOL		**/``	700	1302020	3/19/18
LMCOCHIC		41/44	VOLI	00002829	03/08/78
LMOONAH2C		20/YK		00002830	03/08/18
LMUSEPH2C		03/18	VOLZ PHOT2	00002831	03/08/18
LMJSDPH2C		63/YR	V0L2	00002832	03/08/78
LN74NDH2C		30778	706	33932833	03/38/70
LMD3NDH2C		30/YR	VUL 2	00002834	03/08/78
LMDDAPH2C		26/48	+ 66P VOL3 PHOT3	00002835	03/05/19
S TOLHECCIA		2.2-1/6		66332836	03/13/16
~		5.2-1/GM		00002837	03/13/70
		3.2-17CM		000012838	13/13/18
		M9/1-7.6	# 300 CEFAULT	55870000	03/13/18
		5 2-1/6	# 300 DEFAULT	00002840	03/13/18
S 340H2CC18		5.2-1/GM		00002841	03/13/78
		S 2-1/1:W		2.02000	03/11/10
		S-2-1/6M		60602844	03/13/19
		5-2-1/64		00002845	03/13/18
		5.2-1/GM		00002846	33/13/78
S BADHZCCTH		5.2-7/GM		00002847	03/13/76
		5.2-7/GM	* 300 CEFAULT	00002848	03/13/76
		5.2-7/GM		00012849	63/13/14

	03/13/78	03/13/78	03/13/78	03/13/78	03/13/78	03/13/16	03/13/76	03/13/78	03/13/78	03/13/78	03/13/16	03/13/78	03/13/78	03/13/76	03/13/78	03/13/78	03/13/78	32/13/18	03/13/78	03/13/78	03/13/78	03/13/78	03/13/78	03/13/78	03/13/78	03/13/78	03/13/78	03/13/78	03/14/18	03/14/78	93/14/78	03/14/18	33/14/78	03/14/78	03/14/78	03/14/78	93/14/18	03/14/76
JLE TST18	00002850	00002852	03302854	00002855	00002857	00002858	00000000	00002861	00002862	00002864	00002865	00002866	00002868	00002869	00002870	00002872	00002873	0.90 12875	00002876	00002877	00002879	00002881	00002882	00002883	00002885	00002886	00302888	00002849	000000	00003130	00003140	00003190	00003232	00003203	00003204	00003206	00003237	00003208
LISTING OF MCDULE TSTIB		* 300 CEFAULT	* 300 DEFAULT	* 300 CEFAULT	* 300 DEFAULT		* 300 CEFAULT		* 300 DEFAULT			* 300 CEFAULT			* 300 DEFAULT		* 300 DEFAULT			* 300 DEFAULT * 300 DEFAULT		* 300 DEFAULT		# 30) CEFAULT	-	* 300 CEFAULT		# 300 DEFAULT				* 3.2 DEFAULT	* 3.2	* 3.2	* 3.2	* 3.2 * 3.2	* 3.2	* 3.2 * 3.2
0360																																						
TIME	5.2-7/GM 5.2-7/GM	-2-1/GM	2-1/GM		M9/1-0	-1/6M	17/64	-7/GM	- 1/6M	18/64 18/64	8/6M	-8/6M	-8/6M	8/6M	8/GM	8/6M	¥ 3	E	Σ	EE	Σ	Z Z	25	Z Z	3	¥ 3	¥ 5	E						2	S	.25	5	.25
178	10 10 1					2.	2	~	-2-	8-2-8	->-	2 5	2 2	-2	-2.		1	.2-8/6M	.2-8/GM	.2-8/6M	.2-8/6	.2-8/GM	- 1	.2-8/6M	.2-8/6M	.2-8/GM	.2-8/GM	.2-8/6M	.25	. 25	• 25	.25	.25	. 55	.2	• •		
04/10/78		r u		5.2	2.5	5.2	2	~	5.2-	5.2-8	->-	2	2 2	-5.	2 5		5.2-8/		5.2-8/0	5.2-8/(	5.2-8/GM	5.2-8/	- 1	5.2-8/	5.2-8/	5.2-8/GM	5.2-8/	5.2-8/	.25	.25	.25	•25	.25	.5	ž•			
047E 04/10		v v	5.		2	5.5	2	~	5.2-	5.2-8	->-	2 5	2 2	-2	-2.		1		5.2-8/0	5.2-8/(	5.2-8/6	5.2-6/	- 1	5.2-8/	5.2-8/	5.2-8/	5.2-8/	5.2-8/	.25	•25	. 25	.25	. 25	.5	.2		2.	
		DEBH2CCTR 5		SCPH2CCTx 5.		DNPH2CCTR 5.2	5.5	5.5	5.2	2NTH2CCT3 5.2-8	->-5	2 5	5.5	5.2-	-2.	5.5-	1	-2.5	5.5	TNBH2CCTG 5.2-8/0 CNBH2CCTG 5.2-8/0	CBH2CCTG 5.2-	30PF2CCTG 5.2-8/	5.2-	4NDH2CCTG 5.2-8/ 3NDH2CCTG 5.2-8/	5.2	2ADH2CCTG 5.2-8/		409H2CCTG 5.2-8/				1CP HUM . 25		NTHUM		255FUN 346HUN		T11HUP ENGHUV

	33/14/78	03/14/16	03/14/18	93/14/18	03/14/18	03/14/18	03/14/18	03/14/78	03/14/78	03/14/78	03/14/18	03/14/18	03/14/18	03/14/18	03/14/78	03/14/76	03/14/78	46156130
JLE TSTIB	00003210	00003211	00003212	00003213	00003214	00003215	00003216	00003217	60003218	00003219	00003220	00003221	00003222	00003223	00033224	00003225	00003301	707000
LISTING OF MCDULE TSTIB	* 3.2	# 3.2	* 3.2	* 3.2	* 3.2	* 3.2	* 3.2	* 3.2	* 3.2	* 3.2	* 3.2	* 3.2	# 3.2	* 3.2	* 3.2	* 3.2	* 3.2 DEFAULT	
0560																		
TIME	.25	.25	.25	.25	. 25	.25	.25	.25	.25	.25	.25	.25	.25	.25	.25	.25	.25	
84/101/49																		
DATE																		
NG. 6165	ANTHUM	ANBHUP	ACBFUM	409HUP	BADHUM	ADCHUM	ABDHUM	TNBHUM	CNBHUP	DCBFUP	DNAHUM	30PHUP	SCPHUM	4NDHUM	3NDHUR	DNPHUM	TATHUM	
Z Z	α	α	ď	œ	×	α	œ	α	œ	α	œ	œ	Œ	α	œ	α	¥	

#### Populations, Flows and Travel Times

The line numbers corresponding to these variables are cataloged in Table 2. On each line is the variable, its qualifier subscripts, the variable value (best estimate) and its uncertainty assignment. Information following the uncertainty is either commentary or a document identifier.

TABLE 2. LINE NUMBERS FOR POPULATION DATA, FLOW RATES AND TRAVEL TIMES USED IN COMPUTATIONS

Group	Population Size	Flow Rate	Travel Time
Joliet Humans 1	830	22 <b>6</b> 0	2080
Joliet Fish 1-3	831-833	22 <b>7</b> 0 <b>- 229</b> 0	2090 <b>-</b> 2110
Radford Humans 1	551	2180	2120
Radford Fish 1-4	610-613	2230 <b>-</b> 2233	2170 <b>-217</b> 3
Volunteer Humans 1-2	630-631	2300-2310	2480-2490
Volunteer Fish 1-4	671-674	2350-2380	2530-2560
Holston Humans 1-4	750-780	2580 <b>-</b> 2583	2400-2403
Holston Fish 1-3	800-802	2630 <b>-</b> 2632	2450-2452

Units of N are arbitrary, but must be unique for each population type. SMF may be expressed in either liter/year or  $ft^3/sec = 8.9x10^8$  liter/year). SMT is usually expressed in days.

The actual situations represented by these variables are discussed below and schematically portrayed in Figures 2 through 5.

Joliet Army Ammunition Plant. TNT was tewaters flow to the Illinois River at the juncture of the Des Plaines and Kankakee Rivers. Three fish populations represent fish in three "pools," each formed behind a water regulation dam. Fish populations for this situation (and the others) were computed by methods described in reference 3. The human population represents Peoria, IL. The Illinois River is used as a portion of its water supply; the population size is prorated to reflect the percent of supply from the river.

Radford Army Ammunition Plant. TNT wastewaters flow to the New River. Fish in the New River are divided into four groups. The first three are

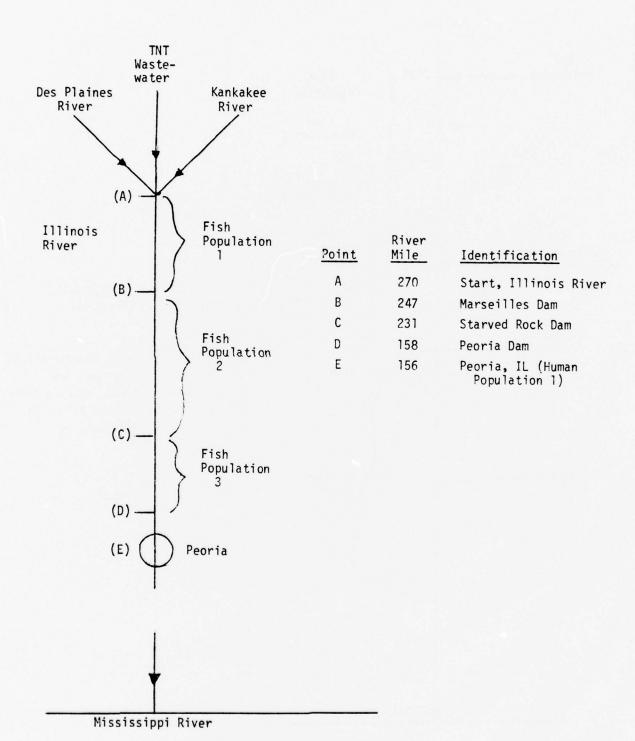


Figure 2. HRAM Representation of Populations at Risk from TNT Wastewaters of Joliet Army Ammunition Plant.

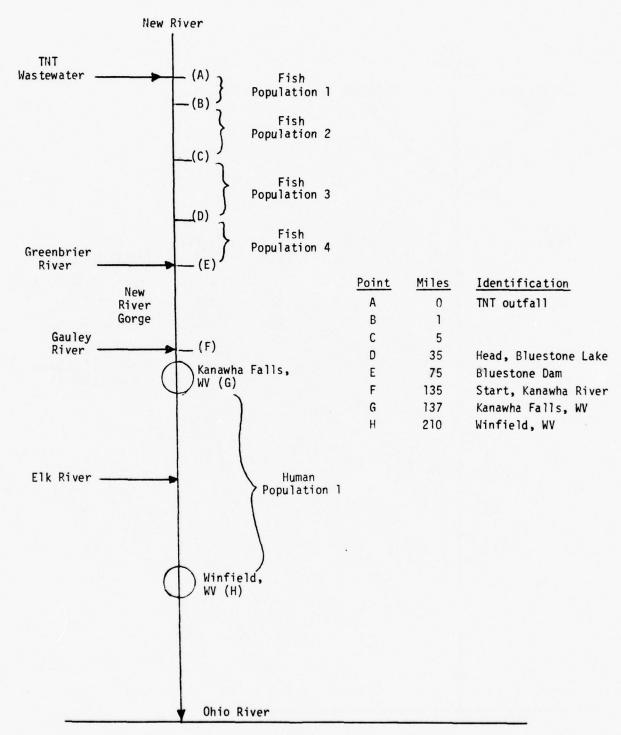


Figure 3. HRAM Representation of Populations at Risk from TNT Wastewaters of Radford Army Ammunition Plant.

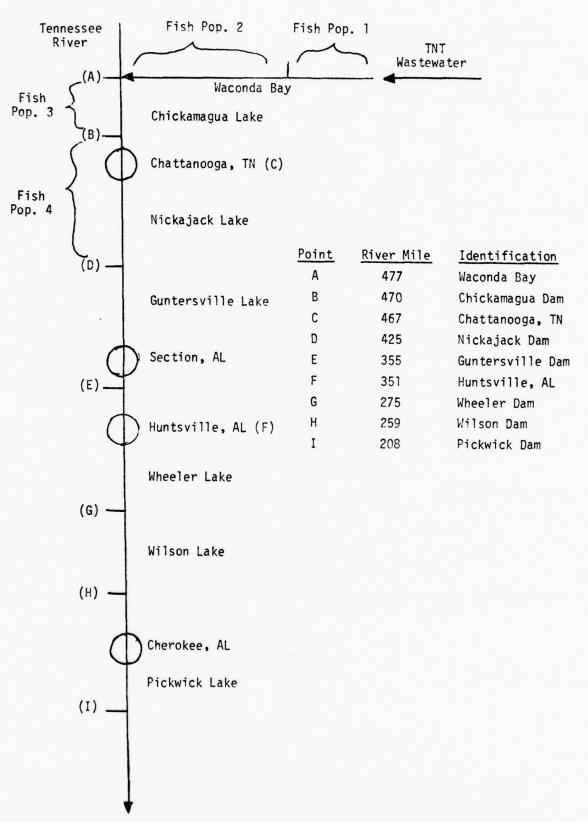


Figure 4. HRAM Representation of Populations at Risk from TNT Wastewaters of Volunteer Army Ammunition Plant.

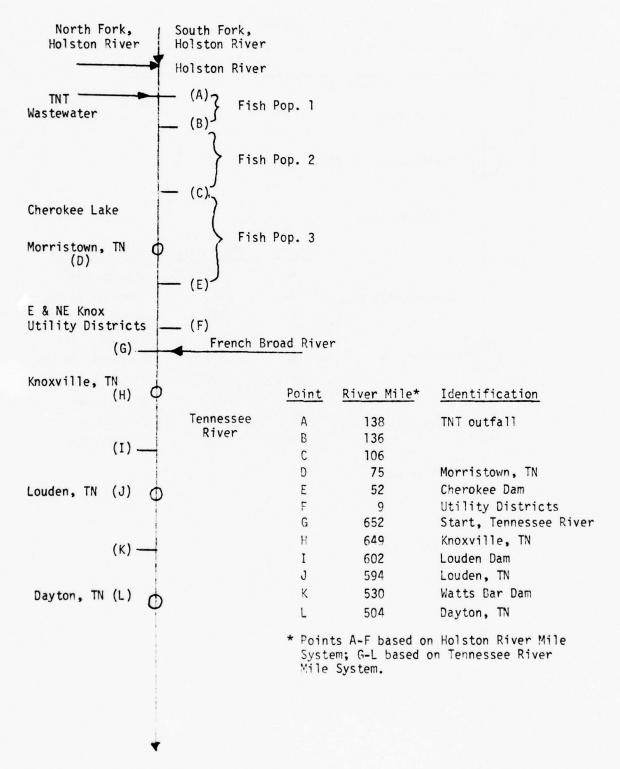


Figure 5. HRAM Representation of Populations at Risk from TNT Wastewaters of Holston Army Ammunition Plant.

based on arbitrary sections of the river, the last group inhabits Bluestone Lake. From the town of Kanawha Falls, WV to Winfield, WV, several utilities serving 70,000 persons use the Kanawha River as their drinking water supply. For these populations, travel time estimates ranged from 4.7 to 6.9 days. To reduce the number of computations without seriously affecting accuracy, these communities were represented as one population group at 5.7 days travel time.

Volunteer Army Ammunition Plant. This is the most complicated and least accurately-defined situation, as reflected in the higher uncertainties assigned to flow and travel times. TNT wastewaters discharge to the head of Waconda Bay. The bay is a backwater of Chickamagua Lake, the reach of the Tennessee River behind the Chickamagua Dam. The only consistent flow to the bay is wastewater from Volunteer Army Ammunition Plant. Considerable time is expected for pollutants to traverse Waconda Bay, although it is only 2 miles long, and to mix with the main stem flow of the Tennessee River.

Two fish populations are specified for the bay. Flow rates are assumed as roughly 4 and 10 times wastewater flow respectively. Travel time is estimated on the basis of section of bay water capacity and flow rate. The fish in Chickamagua Lake below Waconda Bay are considered a third population; the fish in Nickajack Lake are considered a fourth population. The Tennessee River is the water supply source for several Tennessee and Alabama communities. Since the bulk of travel time is expected to occur from the wastewater outfall to Chickamagua Dam, these communities were represented by two population groups. The first represents communities from Chattanooga, TN to Section, AL. The second represents communities from Guntersville, AL to Cherokee, AL. Flow and travel time variables are keyed to the most populous communities in these groups, Chattanooga, TN (158,000 persons) and Huntsville, AL (146,000 persons) respectively.

Holston Army Ammunition Plant. The plant discharges wastewaters to the Holston River below the juncture of the North and South Forks, Holston River. Actual discharges are from several outfalls; for HRAM purposes they are represented as one outfall. The waters from the two forks are poorly mixed for a few miles downstream of their juncture. Hence, the first fish population is assumed to have a flow more representative of the North Fork than the whole river. Fish population 2 represents fish that would reside in the Holston River to the head of Cherokee Lake. The lake is expected to add considerable travel time. This is reflected in the SMT of fish population 3 and of the first human population, the city of Morristown, TN. Human population 2 represents two utility districts that draw water below Cherokee Dam. The city of Knoxville, TN draws water from the Tennessee River (which is considered to start at the juncture of the Holston and French Broad Rivers). The last human population represents smaller towns between Louden and Dayton, TN.

#### Pollution Discharge Rates

Discharge rates to surface waters are at the following line number locations:

for Volunteer - 1730, 1760, 1800, 1831-1857, 2040

for Joliet - 1731, 1761, 1820, 1858-1884, 2041

for Radford - 1810 and 2050

for Holston - 2070

The discharges are based on full capacity operations at the plants. Extensive characterization of "condensate water" discharges has been accomplished for Volunteer Army Ammunition Plant from one 50 ton/day TNT production line. There are six such lines at the plant. On the basis of monthly discharge flow data,  $^5$  a full capacity discharge volume of 1.43x10 liter/year was adopted.  $^\dagger$ 

Concentration data had to be critically reviewed, as the analytical method employed, gas chromatography, can mask the possible presence of some compounds by other compounds. With several compounds, only sporadic presence was observed. Accordingly, for compounds where masking was not expected, all analyses, including zeros, were used to compute an estimated mean concentration. For those compounds where masking was expected, the estimated mean was taken as one-half the average of non-zero analyses. The computed concentrations appear in Table 3. The discharge rates in Figure 1 are the products of the flow and concentrations, with proper unit adjustment.

Of note are the rather large percentages of the dinitrotoluenes, partially nitrated products in TNT production. Their higher concentration illustrates the distillation aspects of "condensate water." Similarly, 1,3-dinitrobenzene occurs in an unusually high percentage, although the precursor benzene is a trace impurity in reagent toluene. The aminonitrotoluenes and amino-dinitrotoluenes would be expected from environmental reduction of the di- and trinitrotoluenes that survive the "sellite" process.

For discharges from Volunteer Army Ammunition Plant, an uncertainty of " \* 3" was assigned to those compounds that were not masked in analysis. This reflected the variability of flow, concentration analysis and scale-up to full operating conditions. For compounds where masking was expected, an uncertainty of " \* 5" was assigned. For discharges at

<sup>&</sup>lt;sup>†</sup> In more typical units, 1.75 gallons of wastewater occur/lb of production grade TNT.

TABLE 3. COMPOUND CONCENTRATIONS USED FOR "CONDENSATE WATER"

Compound	Concentration, mg/liter	Remarks
Toluene	0.057	
2-Nitrotoluene	0.009	
4-Nitrotoluene	0.020	
3-Nitrobenzonitrile	0.001	
4-Nitrobenzonitrile	0.0004	
2-Amino-4-nitrotoluene	0.006	
2-Amino-6-nitrotoluene	0.017	Masked
3-Amino-4-nitrotoluene	0.001	
3-Methyl-2-nitrophenol	0.011	Masked
5-Methyl-2-nitrophenol	0.068	Masked
1,3-Dinitrobenzene	2.05	
2,3-Dinitrotoluene	0.198	Masked
2,4-Dinitrotoluene	7.26	Haskea
2,5-Dinitrotoluene	0.111	
2,6-Dinitrotoluene	3.55	
3,4-Dinitrotoluene	0.192	
3,5-Dinitrotoluene	0.180	
3,5-Dinitroaniline	0.004	
1,3,5-Trinitrobenzene	0.076	Masked
2,3,6-Trinitrotoluene	0.134	Masked
2,4,6-Trinitrotoluene	0.482	Masked
2-Amino-3,6-dinitrotoluene	0.002	
2-Amino-4,6-dinitrotoluene	0.012	Masked
3-Amino-2,4-dinitrotoluene	0.431	Masked
3-Amino-2,6-dinitrotoluene	0.288	Masked
4-Amino-2,6-dinitrotoluene	0.269	Masked
4-Amino-3,5-dinitrotoluene	0.062	
5-Amino-2,4-dinitrotoluene	0.549	
2,4-Dinitro-5-methylphenol	0.043	Masked
1,5-Dimethy1-2,4-dinitrotoluene	0.116	

Joliet Army Ammunition Plant, uncertainties of " \* 5" and " \* 7" were respectively assigned. These increased uncertainties account for extrapolations made between plants.

TNT discharges at Radford Army Ammunition Plant are two-thirds of the estimated discharges that existed prior to production stoppage due to an explosion. Three 50 ton/day lines then operated; two are to operate when production resumes.

Discharges of 2,4-dinitrotoluene at Radford Army Ammunition Plant are expected to be predominately associated with propellant production rather than with TNT production. Reduced TNT production is not expected to impact on the discharge rate.

TNT discharges from Holston Army Ammunition Plant are the least accurately defined. Plant data<sup>6</sup> indicates discharge rates 10 times higher than used here, but in-river measurements<sup>7</sup> indicate that much lower amounts are present in the Holston River.

#### Environmental Disappearance Rate Constants

Values of LMD are identified by line numbers 2660-2835. This factor tries to typify environmental processes that remove or destroy a compound in terms of first order kinetics. First order kinetics, at least over a short time scale, is a fair descriptor of certain environmental processes. Whether this is accurate over the travel times encountered in this HRAM analysis is not known.

For estimation purposes, several sets of test data or estimates were available from studies performed as part of SRI, International contract efforts. The "roof-top" test<sup>8</sup> was considered the most reliable source of data. In this test, a compound was placed in aqueous solution in two open beakers. The beakers were placed on a roof-top, where they were exposed to diurnal conditions. However, one beaker was shaded. Both beaker contents were stirred. Evaporated water losses were replaced prior to withdrawing samples for analysis. By analysis, the loss of compound by combined photolysis and vaporization or by just vaporization could be measured. From the difference in pseudo-first order loss rates, the photolysis component could be estimated.

Table 4 identifies the compounds that were tested by this method. The results for 2,4-dinitrotoluene are presented in Figure 6 as an illustration. The pseudo-first order rate constant for the summed processes was computed as 49/year; and for the vaporization process, 21/year. Since rates are additive, the photolysis rate constant was estimated as 28/year.

TESTS ON ENVIRONMENTAL EFFECTS FOR TNT WASTEWATER COMPOUNDS AND SELECTED RATE CONSTANTS TABLE 4.

Compound	Roof-Top Test	Photolysis Reactor	Rate Constants, year Vaporization Photoly	ts, year -1 Photolysis
2-Nitrotoluene		×		
4-Nitrotoluene		×		
2,3-Dinitrotoluene	×		30	18
2,4-Dinitrotoluene	×	×	21	28
2,5-Dinitrotoluene	×	×	42	198
2,6-Dinitrotoluene	×	×	49	163
3,4-Dinitrotoluene	×	×	16	4
3,5-Dinitrotoluene	×	×	21	6
1,3-Dinitrobenzene	×	×	16	4
3-Methyl-2-nitrophenol		×		
5-Methy 1-2-nitrophenol		×		
2-Amino-4-nitrotoluene		×		
2-Amino-6-nitrotoluene		×		
3-Amino-4-nitrotoluene		×		
3-Amino-2,4-dinitrotoluene	×	×	-	10
3-Amino-2,6-dinitrotoluene	×	×	20	220
4-Amino-3,5-dinitrotoluene	×	×	6	17
4-Amino-2,6-dinitrotoluene	×	×	9	183
5-Amino-2,4-dinitrotoluene	×	×	2	12
1,5-Dimethyl-2,4-dinitrotoluene	×	×	56	64

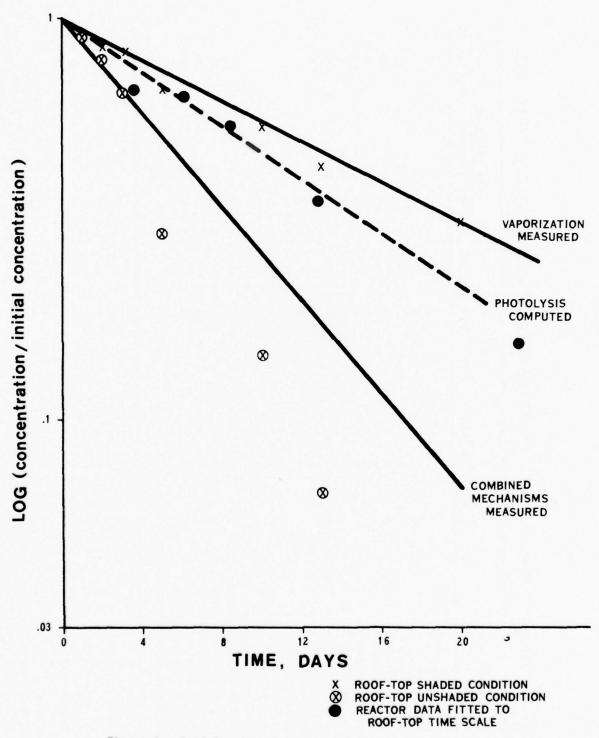


Figure 6. Roof-Top Test Data and Photolysis Reactor Time Estimates for 2,4-Dinitrotoluene.

LMD was then computed by the following assumed relation:

LMD = 2/3 (vaporization rate constant) + 2/5 (photolysis rate constant) (6)

The fractions were applied to adjust for less effective sunlight or cooler average weather conditions in actual environments. The test was performed in Menlo Park, CA in the summer, during a period of clear, sunny days.

When not available from the "roof-top" test, photolysis data were derived from results of another test apparatus, the flow-through photolysis reactor. The aqueous solution flowed through a glass coil. A tubular irradiation light was placed along the coil axis. The arrangement was placed in a thermostatically controlled water bath. Flow rate through the coil, and hence exposure time, was controlled.

For reactor results to provide constants comparable to those from the "roof-top" test, common 2,4-dinitrotoluene test results were used for adjustment. Figure 6 shows these results superimposed along the estimated photolysis curve. Most other compounds that had been tested both ways agreed reasonably well with this adjustment of time. Table 4 also indicates the compounds analyzed with the reactor. The photolysis data used are in reference 9.

For other vaporization rate constants, Spanggord<sup>10</sup> provided rough estimates based on gas-chromatograph retention times. These were converted to rate constants on the basis of a side-by-side comparison of those compounds for which both "roof-top" and gas chromatograph data were provided.

For toluene, the methyl-nitrophenols, the nitrobenzonitriles and 1,3,5-trinitrobenzene, photolysis was considered unimportant in computing LMD. For TNT and 2,3,6-trinitrotoluene, vaporization was considered unimportant. Moreover, photolysis rates equal to that of 2,6-dinitrotoluene were adopted, based on a suggestion by Barkley. For any remaining compounds, a default LMD of 20/year was used.

Table 4 shows vaporization and photolysis rate constants for several compounds. The striking feature is the wide range of photolysis constants within an isomeric group. From structural considerations, the 2,6-dinitro configuration promotes photolytic degradation. However, other generalizations are not apparent.

Uncertainty assignments for these LMD were an involved process. The term exp(-LMD \* SMT) poses a problem to the assumption of log-normal hazard. If LMD is assumed log-normal, and the uncertainty contribution from SMT of minor importance, the stochastically-computed hazard consistently underestimates the deterministically-computed hazard. The larger

the uncertainty, the larger the skew. Use of a percentage uncertainty for LMD was found to largely avoid this bias.

An <u>ad hoc</u> method of quantifying uncertainty had to be developed. Consideration was given to the 95 percent range expected to exist for  $\exp(-LMD * SMT) = 0.001$ . For LMD data considered the most accurate (a roof-top test with good agreement with reactor results), a 100-fold range was assumed due to LMD uncertainty. From this, an uncertainty of "+ 33 P" was calculated. For the poorest quality LMD data (default), the range was assumed to be 10,000-fold. This corresponded to an uncertainty of " + 66 P." Other percentages were intermediate based on the quality of the data sources.

## Retention Factors

These factors are listed on line numbers 3090-3301. All values are set to 0.25 with an uncertainty of " \* 3.2." Compounds in the environment, even at concentrations below their aqueous solubility, do not exist solely in solution. They would be adsorbed on living or mineral particulate matter in river or lake water. Water treatment processes remove such matter, reducing the amount of compound available for human ingestion. The value 0.25 is considered typical of such treatment processes.

#### Concentration-Dose Conversion Factors

Values of SMB for chronic human dosing is 500 liter/year, representative of a yearly level of consumption. The dose-risk slopes for several chronic effects from several compounds (line numbers 2836-2889) have the SMB factor incorporated in cgs units, 0.0159 cc/sec. Since this factor is assumed invariant, this is allowable.

#### Effects and Values

Five effects are considered in this study. Effects to humans are considered only from chronic dosing. The effects are:

- 1. Some mutagenic or carcinogenic response in humans (C). This is valued at \$300,000 per occurrence.
- 2. Some severe non-mutagenic or non-carcinogenic effect in humans (CTG). This could mean outright death or other response that would be considered of socioeconomic equivalent. This is also valued at \$300,000 per occurrence.
- 3. Some mild response in humans (CTR). This would be equivalent to toxic responses that are noted in long-term studies in mammals where CTG-type effects are not observed. This is valued at \$30,000 per occurrence.

- 4. Fish kill due to acute exposure (FKL). This is an episodic effect expected to occur once yearly during a period of low flow. This is valued at \$1.00 per fish killed. This is derived on a per weight basis.
- 5. Chronic fish effect (CFS). This is an effect manifested due to continual contact with a pollutant in water. Some examples would be loss of reproductive ability, death or tainted flesh. This is also valued at \$1.00 per affected fish.

These effects are purposely vague. When detailed data is not available about compounds, it is difficult to predict specific effects.

Moreover, different compounds will manifest different effects which are of equivalent adverse value.

## Dose-Risk Slopes

Fish Effects. Line number locations for these data are as follows:

#### Compound

1200, 1207
1253, 1256
1322, 1327
1291, 1292
1281, 1282
1330-1390

The valuations are based on bioassay screening tests performed by SRI, International and summarized in reference 12. The lower of either the 48-hour EC50 to Daphnia $^{\dagger}$  or the 96-hour LC50 $^{\dagger\dagger}$  to a fish species was the basis for slope determination. The slopes and uncertainty assignments were determined as described in reference 3:

$$S(FKL) = 0.1/LC50 \text{ (or EC50), uncertainty} = *4$$
 (7)

$$S(CFS) = 3 * S(FKL)$$
, uncertainty = \* 15 (8)

The notation S(mnemonic of effect) will be used as a shorthand notation in subsequent sections of this report.

This is the statistically computed concentration of that which will cause death to 50 percent of fish after 96 hours exposure.

This is the statistically computed concentration of that which will cause death (or the observable equivalent) to 50 percent of Daphnia after 48 hours exposure.

<u>Human Effects.</u> Line number locations for these dose-risk slopes are cataloged in Table 5. For the carcinogenesis effect, the value for 2,4-dinitrotoluene is based on results of a 2-year mammalian (rats) study by Ellis, et al.  $^{13}$  Tumors were not observed in test animals which had been dosed with 5 mg/kg/day or less of 2,4-dinitrotoluene. This was the first data available based on such a study. Conversion to HRAM format was based on an adaptation of a method reported by Hoel, et al.  $^{14}$  First, an adjusted human equivalent dose (AHED) is computed.

AHED = Animal dose \* (Human weight/animal weight)
$$^{2/3}$$
 (9)

For 0.4 kg rats and 60 kg humans, a dose of 140 mg/day or 51 g/year is computed.

TABLE 5. DOSE-RISK SLOPE DATA LINE NUMBER LOCATIONS

Compound	S(C)	S(CTR)	S(CTG)
2,4,6-Trinitrotoluene	1180	1203	1205
2,4-Dinitrotoluene	1250	1254	1252
4-Amino-2,6-dinitrotoluene	1280 (	see below, othe	r compounds
2-Amino-4,6-dinitrotoluene	1290 (	see below, othe	r compounds
2,6-Dinitrotoluene	1320	1324	1 321
"Condensate water"	1 3 6 0	1362	1361
Other compounds	1461-1485	2836-2862	2863-2889

Given the number of animals tested, determine an upper 95 percent confidence limit on the range of the "true" risk at the highest observed "no-effect" level. This is a consequence of binomial distribution statistical arguments; tables and graphs are available for this purpose. For 120 test animals, this limit is 0.04.

The log-normal uncertainty is chosen that would be applicable to the data at the current state of knowledge. The confidence limit determined above is divided by this uncertainty. In this case, an uncertainty of "\* 10" is chosen, which is somewhat higher than that which would be assigned if the test had involved two mammalian species (see Research Projects, page 46). This value is 0.004.

The dose-risk slope is that of the line that passes through the dose-risk origin and the point (AHED, upper 95 percent confidence  $\frac{1}{5}$  uncertainty). In this case, the result is 0.004/51 or  $8\times10^{-5}$ /gram.

All other compounds except "condensate water" have been processed through an Ames/Salmonella mutagenic bioassay by SRI, International. This bioassay determined the mutgaenic activity of compounds to five mutant strains of Salmonella typhimurium: TA 1535, TA 1537, TA 1538, TA 98 and TA 100, in the presence and absence of a rat-liver activation system. These bacteria are not expected to survive in the nutrient medium supplied (with compound addition) unless they revert to a normal state through mutation. Some do revert without any compound addition; this condition serves as the bioassay control. If increasing amounts of a compound cause an increasing number of reversions, the compound is deemed to have mutagenic potential. If this occurs with the activation system, metabolites of the compound have mutagenic potential. If the compound fails to cause significant reversions with all strains with and without activation, the compound may not be mutagenic.

The results of these bioassays have been reported in reference 8. The investigators also determined a potency factor, which is the maximum number of revertants/microgram of compound for the most pronounced strain-activation situation. A maximum exists because a compound, above a certain mass level on a plate, becomes toxic. These potency factors have also been reported.<sup>8</sup>

The potency factor has not been accepted by the scientific community as immediately translatable to a mammalian system. However, it did appear worthy of some weighting since a life system was involved and 2,4-dinitrotoluene, for which more detailed testing had been done, was also processed through the bioassay. Accordingly, the following relation was used to compute S(C) for compounds with mutagenic potential:

 $S(C) = 8 * 10^{-5}$  (potency of compound/potency of 2,4dinitrotoluene)<sup>2/3</sup> (10) An uncertainty of " \* 20" was assigned to all such S(C).

The compounds observed not to have mutagenic potential were toluene, 2-nitrotoluene, and the methyl-nitrophenols. Since the bioassay is not a perfect predictor, some probability exists that they may have mutagenic potential. The values adopted for their S(C) were based on "activity tree" procedures described in reference 3. An uncertainty of " \* 20" was also assigned. The estimated S(C) for "condensate water" was determined on contributions from its major constituent on the basis of concentration.

Estimates of S(CTR) and S(CTG) had been previously determined for TNT, 2,4-dinitrotoluene and 2,6-dinitrotoluene. Estimates for "condensate"

water" were made on the basis of these, adjusted for concentration contributions. Somewhat higher uncertainties were assigned to S(CTG) and S(CTR) for "condensate water" than for the other three compounds. For all other compounds, the default slopes and corresponding uncertainties suggested in reference 3 were used. These slopes are: S(CTR) =  $3.3 \times 10^{-5} / \text{gram}$  and S(CTG) =  $3.3 \times 10^{-6} / \text{gram}$ . The SMB has been incorporated into these values in the data base.

## HAZARD ANALYSIS AND DISCUSSION

The data base of Figure 1 was processed to compute hazard. This was done in part to present such data for the meeting, and to determine which research projects to consider in the allocation analysis. The same program is used for hazard and allocation. For hazard, the data inputs are altered as follows:

- a. All uncertainties are reset to near certain levels (\* 1.001).
- b. One research project is inserted which forces reevaluation of all hazards computed by Equation (2). The section on Research Projects discusses this in more detail.
  - c. Two Monte-Carlo simulations are performed.

A portion of the print-out is shown in Figure 7, which shows the data and computations corresponding to Equation (2). These hazards can be summed by location and population subgroup to indicate the hazards computed in Equation (3). Table 6 is the hazard summary for those compounds with hazards of 100 or greater. Other compounds with hazards of one or greater were:

3-amino-2,4-dinitrotoluene	91
2-amino-4,6-dinitrotoluene	42
2,5-dinitrotoluene	41
4-amino-2,6-dinitrotoluene	34
3-amino-2,6-dinitrotoluene	32
3,5-dinitrotoluene	16
2,4-dinitro-5-methylphenol	16
1,5-dimethy1-2,4-dinitrotoluene	14
3,5-dinitroaniline	14
4-amino-3,5-dinitrotoluene	7
2-amino-3,6-dinitrotoluene	3

<sup>†</sup> Prior to the run, it was anticipated that human effect's hazards would be numerically low. To improve precision, execution was accomplished with an (R) of 2.5 for humans. Figure 7 shows the print-out under this condition.

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Figure 7. Hazard Computations Corresponding to Equation (2).

TABLE 6. HAZARD BY COMPOUND AND EFFECT (PARTIAL LIST)

Compound	Human Effects CTR + CTG	fects C	Human Total	Fish Effects CFS + FKL	Total for Compound
"Condensate water"	16	153	169	2173	2342
2,4,6-Trinitrotoluene (all)	100	594	694	2333	3027
2,4,6-Trinitrotoluene (in condensate water)	2	14	16	132	148
2,3,6-Trinitrotoluene	-	12	12	992	778
2,4-Dinitrotoluene (all)	39	145	184	332	516
2,4-Dinitrotoluene (in condensate water	25	84	109	279	388
1,3-Dinitrobenzene	4	82	98	410	496
5-Amino-2,4-dinitrotoluene	2	19	21	467	488
3,4-Dinitrotoluene	~	2	5	185	190
1,3,5-Trinitrobenzene	~	31	31	113	144
2,3-Dinitrotoluene	~	4	4	122	126
2,6-Dinitrotoluene	2	80	10	93	103

The print-out in Figure 7 also shows risk, which in terms of variable notation is:

$$Risk = C * S * SMB \tag{11}$$

Hazard ranking is indifferent to situations of high risk-low population as opposed to low risk-high population. An allocator may have more interest in the former situation.

Fish risks are highest for Volunteer fish population 1, which is not surprising, given its travel time and flow variables. However, the larger-sized fish populations assigned at Joliet cause that plant to contribute the greatest increment to hazard. Conversely, for humans, the greatest risk is at Joliet, but due to population size, the greatest hazard increment is from Volunteer.

Table 7 is a partial listing of computed risks, taken for the most exposed population. The correspondence between these risks and hazards in Table 6 is not perfect. For example, the hazard of 1,3,5-trinitrobenzene to fish is higher than that of 2,6-dinitrotoluene. Yet, the risk of the most exposed fish group to 1,3,5-trinitrobenzene is lower than that to 2,6-dinitrotoluene. This apparent anomaly is due to the different LMD. The 1,3,5-trinitrobenzene is more persistent. Hence, it poses a lower risk to fish populations at small travel times, but would pose a relatively higher risk to fish populations at more distant travel times.

The sensitivity of hazard values to LMD is illustrated by a hypothetical example. The data base is in Table 8. All information required for Equation (2) is included with the exception of LMD. Table 9 presents the computed hazards with this data and different values of LMD. The greatest changes occur with the most time-distant populations, which would be expected from the exponential term. While the example is contrived, it does illustrate some important features of the TNT wastewater situation. Populations are located at travel times that are relatively short and long. Thus LMD assignment, barring gross mismatches, is probably not a decisive factor in the sensitivity of hazard results. The example shows that such a conclusion is a function of the demographic features of the situation.

The hazard results consistently show that the hazard to fish would be of more concern than to humans. Given the time-distance and size of fish populations, this is not totally unexpected. The vulnerability of fish as compared to humans, as seen in Table 7, overshadows the larger premium that is placed on human effects. This is indicative of a trend noted with compounds that have undergone extensive toxicological testing and for which some recommendations for standards have been prepared; the aquatic toxicology has been the most stringent criterion.

TABLE 7. RISKS ASSOCIATED WITH COMPOUNDS FOR THE MOST EXPOSED POPULATIONS (PARTIAL LIST)

	Human E	ffects	Fish Effect
Compound	CTG	С	CFS
"Condensate Water"	5.6x10 <sup>-10</sup>	1.1x10 <sup>-8</sup>	1.1x10 <sup>-2</sup>
2,4,6-Trinitrotoluene <sup>a</sup>	2.3x10 <sup>-9</sup>	2.8x10 <sup>-8</sup>	1.3x10 <sup>-2</sup>
2,3,6-Trinitrotoluene	1.8x10 <sup>-12</sup>	9.4x10 <sup>-10</sup>	4.8x10 <sup>-3</sup>
2,4-Dinitrotoluene	1.9x10 <sup>-10</sup>	5.1x10 <sup>-9</sup>	$1.5 \times 10^{-3}$
1,3-Dinitrobenzene	7.6x10 <sup>-11</sup>	3.5x10 <sup>-9</sup>	1.9x10 <sup>-3</sup>
5-Amino-2,4-dinitrotoluene	2.3x10 <sup>-11</sup>	6.0×10 <sup>-10</sup>	1.6x10 <sup>-3</sup>
3,4-Dinitrotoluene	7.0x10 <sup>-12</sup>	1.7x10 <sup>-10</sup>	$8.9 \times 10^{-4}$
1,3,5-Trinitrobenzene	3.0x10 <sup>-12</sup>	1.0x10 <sup>-9</sup>	5.3x10 <sup>-4</sup>
2,3-Dinitrotoluene	5.6x10 <sup>-12</sup>	2.4x10 <sup>-10</sup>	$6.5 \times 10^{-4}$
2,6-Dinitrotoluene	4.1x10 <sup>-11</sup>	6.5x10 <sup>-10</sup>	$6.2x10^{-4}$

a. Maximum human risk at Radford Army Ammunition Plant; maximum fish risk at Holston Army Ammunition Plant.

TABLE 8. HYPOTHETICAL DATA BASE TO ILLUSTRATE SENSITIVITY OF HAZARD TO LMD

Population Data, Flow Rates, and Travel Times

	Size	Flow Rate (liter/year)	Travel Time (days)
Human 1	50,000	3x10 <sup>12</sup>	3
Human 2	250,000	1×10 <sup>13</sup>	40
Fish 1	20,000	1×10 <sup>10</sup>	1
Fish 2	5x10 <sup>6</sup>	5×10 <sup>12</sup>	25

Discharge rate - 20,000 kg/year

Effects Data

Effect	Slope
CTR	8x10 <sup>-5</sup> /gram
CTG	5x10 <sup>-6</sup> /gram
С	2x10 <sup>-4</sup> /gram
CFS	0.33 liter/mg-year
FKL	0.10 liter/mg-year

 $\mbox{\sc Values}$  , water treatment retention, and concentration-dose conversion factors are the same as in analysis.

TABLE 9. HAZARDS FROM TABLE 8 DATA BASED ON DIFFERENT VALUES OF LMD

		Hazard for S	pecified LMD	
	LMD=10	LMD=20	LMD=50	LMD=100
	<u>н</u>	umans		
Population 1 Population 2	2453 1334	2259 446	1765 17	1170 0
Total	3787	2705	1 782	1170
		Fish		
Population 1 Population 2	16851 4365	16397 2201	15103 282	13169 9
Total	21216	18598	15385	13178
Grand Total	25003	21303	17167	14348

Another consistent result is that the mutagenic potential predominates over other chronic effects in humans. This may be an artifact, in that very different approaches are taken to develop dose-risk slope values for these effects.

Tables 6 and 9 have neglected to show the units of hazard, nominally in dollars/year. This is deliberate. There is a tendency to take dollar amounts at face value or to misinterpret them. The reader is reminded that most of the concepts used in data base preparation are untested and quite empirical.

#### THE ALLOCATION ANALYSIS

## Research Projects

Based on the computed hazards, a truncated set of research projects were selected for allocation analysis; they appear in Figure 8. The compounds are those with hazards of 100 or greater. With the exception of TNT, 2,4-dinitrotoluene, 2,6-dinitrotoluene, and condensate water, all compounds had the same demographic factors (N, SMF, SMT) and the same uncertainty assignments for dose-risk slopes. Thus, by comparison through hazard, the allocation objective factors for the other compounds could be inferred.

Each line entry consists of:

- a. The mnemonic code "PRO"
- b. A three character mnemonic of the project title.
- c. The variable whose uncertainty is to be reduced.
- d. The variable subscripts. These are supplied in fixed order. Some latitude is available in their use. The most restrictive approach would be the subscripts associated with the variable in the data base. The notation "XXX" or "ALL" is used to signify that a variable is not applicable or is not a restriction. Thus, the first project shown in Figure 8 causes all contributions to hazard that include any variable N to be computed. This is, of course, what is desired to produce the hazard ranking.
  - e. The research cost.
  - f. The expected uncertainty after the research project is done.
- g. Space to describe the project or documentary information. This is for user convenience.

Project "AAT" is an acute toxicity test for aquatic species. It includes more species, duration of tests, effects observed, and animal physiology than in the completed screening studies. The project is expected to cost \$20,000 per compound. It is expected to reduce the uncertainties associated with S(CFS) and S(FKL). Project "LTM" involves a detailed 2-year chronic feeding study of several mammalian species. Intensive pathology and physiology is performed, with special attention to the incidence or tumors or other abnormalities that could be considered precursors of carcinogenicity. The project is expected to cost \$400,000 per compound. It is expected to reduce the uncertainties associated with S(CTR), S(CTG) and S(C).

A project "LTM" for 2,4-dinitrotoluene was not included, as such a study has been completed. A "LTM" project is underway with TNT, but since the data base is "pre-LTM," the project was included for post-decision analysis.

# Statistical Considerations of the Allocation Methodology

The next section will review in some detail the aspects of the generation, assembly and interpretation of objective factor results. As this is the first full exercise of HRAM, these facets are of interest. There are aspects of the analysis which may be more artifacts of the algorithms rather than valid conclusions. There may be pitfalls to placing too much reliance on a set of objective factor results.

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1	34 DXX XH2UXXXXXX FKL	20*	-	AQUATIC	STUDY		001072	03/13/78
	TNBXXXHZUXXXXKKL	*07	PHASE I	AQUATIC	STUDY		001013	03/13/78
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	UNBXXXHZOXXXXXCTR	*00*	3 TWO YEAR MAMMAL	MAMMAL	STUDY		00101	02/22/78
	340XXXHZOXXXXXCTR	*005		MAMMAL	STUDY		001018	02/22/78
PRULIMS ABOXX	ABDXXXHZOXXXXXCTK	*004	3 TWO YEAR MAMMAL STUDY	MAMMAL	STUDY		00100	02/22/78
	ABDXXXXXXXXCTG	*00*		YEAR MAMMAL STUDY	UDY		180100	02/22/78
	TNBXXXH20XXXXXCTG	*005	YEAK	ž .	STUDY		001082	03/13/78
PRULIMS 340XX	34 DXX XHZOXXXXXX CTG	*005	YEAR	MAMMAL SI	STUDY		001083	02/22/78
	INTXXXH2CXXXXXCTG	*00*	7 2 YEAR M		STUDY		001084	02/22/78
PROLIMS TCPX	TCPXXXH20XXXXXCTG	*005	YEAK	MAMMAL ST	STUDY		001086	02/22/78
1	ABDXXXH2UXXXXXXC	*00*	YEAR		STUDY		001087	02/22/78
PRULIMS TOPX)	CPXXXH20XXXXXC	*005	7 2 YEAR M	MAMMAL SI	STUDY		001088	03/14/78
	DNBXXXH2UXXXXXXC	4004	100		STUDY		060100	03/14/78
PROLIMS 340XX	34DXXXH2DXXXXXXC	*005		AMMAL SI	STUDY		160 100	03/14/78
	TNBXXXHZOXXXXXC	<b>*</b> 005	7 2 YEAR MAMMAL STUDY	AMMAL ST	YOU.		001005	03/14/78
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Figure 8. Research Projects for Allocation Evaluation.

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	03/13/78	03/13/78	03/14/78	03/14/78	03/14/78	03/14/78	03/14/78
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These problems are a consequence of HRAM algorithms and statistics. The hazards that are of interest correspond to Equation (3). They are assumed to be log-normally distributed. This assumption is sufficient to allow for the computation of hazard and uncertainty by stochastic methods. The validity of the assumption must be validated by other methods. A set of hazard data will be so treated.

Statistics indicate that theoretical problems may exist with the log-normal distribution assumption. A continuous probability distribution which is the sum of other distributions tends to approach a normal distribution. The more sums involved, the closer is the approach. With most compounds involved here, fish effects involve seven summations; human effects, three. These are probably not large numbers of summations to be of concern. HRAM can, at least in principle, process research projects that involve hazards corresponding to Equation (4). In practice, the interpretation of such results to hazards corresponding to Equation (3) may be difficult. This will be illustrated.

A fundamental concept of statistical sampling (which the Monte-Carlo method simulates) is to provide an estimate of a statistical parameter. The larger the number of simulations, the better the reliability of the estimate. However, a limit must be set, because computer time is involved. For the analysis at hand, each simulation involves 620 computations of Equation (2). With the IBM 360/50 computer, 100 such simulations require 36 minutes. The ramifications of selecting a given number of simulations will be discussed in the next section.

An important consideration involves the credence attached to an objective factor when compared to another. This is complicated by the multi-variable impact of research projects. The objective factor is:

Factors common to several variables (2 for "AAT," 3 for "LTM") are summed to provide overall objective factors for allocation considerations. If each factor was exact, this would cause no concern. However, this is not the case. H is an estimate of a mean hazard; U is the computed estimate of an exact uncertainty. If one takes products, then differences, and next sums, the factor can be rather inexact. An approach to resolve this problem will be discussed.

## Allocation Results and Discussion

The allocation results after one 300 Monte-Carlo simulation run appears in Figure 9. Each line is read as follows:

- 1. The order of analysis.
- 2. The project mnemonic.

1				-	The same of the sa						
-	;	!	1 !!	TYP 10x	HAZARD	UNCERT	HAZARD	UNCERT	DEL HU	DCLLARS	**
€	S	480	H20		309.55	15.19	318.90	8.99	19461		
2 14T		TNB	Н20	CFS	110.91	23.71	110.011	12.70	1216	. 20.	
	S	349	Н 20		171.34	23.52	166.77	11.79	1982		
4 CAT	S	240	Н20		283.94	17.30	286.64	9.36	2265.		_
	S	SNC	н20		416.27	19.72	395.09	9.34	4209		
6 A1T	5	TNT	H20		2304.50	19.61	2286.52	96.6	22300.		1114.579
•1	S	TCP	H20	CFS	2118.22	20.55	2033.41	10.35	21172		_
8 2AT	S	100	н20		635.87	8.68	623.03	5.46	2025		
TF: 6		TNT	H 20	FKL	713.11	6.95	131.99	3.96	2157.		107.858
0 247	2	SNG	Н20	FKL	123.72	96.9	122.37	4.46	307		
TEV 1	S	240	H20	FKL	91.86	1.69	97.32	4.22	339		-
Z AAT	67	340	H20	FKL	50.11	7.66	51.11	5.35	117		
3 A4T	S	TNB	Н20	FKL	35.23		35.62	6.16	85.		4.25
4 . 47	S	480	Н20	FKL	126.20	7.54	123.29	49.4	362		18.12
5	s	TCP	H 20	CTR	60.6	82.24	8.53	9.14	. 449		19.1
W 1 9		TNT	Н20	CTR	52.86	51.73	50.67	2.96	2369,	.004	5.92
		ONB	H 20	CTR	2.18	434.90	2.21	7.58	938.		2.34
8 1.		340	H20	CTR	9.24	374.22	3.22	6.74	83		0.20
_	5	TNB	H20	CTR	0.09	357.29	0.11	9.18	34.		0.086
ב'		480	H20	CTR	0.86	324.87	1.02	7.44	298,	.004	0.74
ר		480	Н 20	CTG	1.26	484.99	1.12	10.67	566.	.004	1.41
2 LTM		TNB	H20	CTG	01.0	362.32	0.11	15.18	36.		60.0
-		340	HZD	CTG	3.28	261.44	0.23	8.52	49		0.161
-		9NG	Н20	510	2.61	344.23	2.34	10.04	827.		2.06
25 LTM		LNL	Н20	510	53.08	36.45	51.54	10.00	1384		3.45
		1CP	H 20	210	1.94	.51.07	8.11	14.91	290.		0.12
٦.		A 8.0	H20	U i	21.19	30.23	27.87	12.07	206.		1.26
		40	H20	J	186.31	46.76	178.28	15.53	5693	-	14.23
_		LN	Н20	O	615.74	39.52	06.809	14.51	15314.		38.28
2		DN9	H20	J	103.07	31.12	102.46	13.17	1866.		4.66
_		340	H20	U	4.34	56.24	19.4	12.56	61.		0.15
Z LIM		TNP	H20	3	36.32	35,89	36.45	15.09	151		1.89
_		111	H20	CTR	0.02	338.34	0.02	16.93	• 9		0.014
4 1.4		11	H20	010	9.32	344.37	0.02	21.27	. 0		0.0
_		11	н 20	S	66.63	38.43	10.40	20.20	185.	.004	0.463
36 LTM	2	760	H20	CTR	1.25	19.05	1.24	11.35	10.	.005	0.05
-		260	H20	CTG	0.53	17.71	0.53	17.71	•		0.0
. L .		692	H20	ی	1.52	33,95	7.61	16.68	131.	4	0.32
39 447	5	Ξ	H20	CFS	587.98	24.21	595.93	13.51	6335.		316.74
14		111	H20	FKL	208.25	10.81	206.52	7.11	769.		38.43
15	· ·	592	H 20	CFS	42.71	23.28	80.57	11.94	956.	. 20.	46.278
7		197	13.00 H	1 L	47.67	11.48	24.16	6.13	48.		2.40
		252	RH		37.96	11.6	37.66	7.14	100.		4.97
		630	H20	CFS	111,82	27.19	112.09	15.02	1350		67.51
40 118	<i>n</i> •	230	120	x (		482.64	0.11	12.05	15	•	0.12
, .	,	2.50	120	5	01.0	21.100	11.0	70.30	66	-076	71.0
ر	0	116/									•

Figure 9. Allocation Data from a 300 Monte-Carlo Simulation Run.

\* INDICATES A GENCVED NEGATIVE DELTA SIGNA.

- The variable with appropriate subscripts whose uncertainty is reduced.
- 4. For the current situation ("prior"), the hazard and hazard uncertainty associated with the variable.
- 5. For the projected situation after research, the corresponding hazard and hazard uncertainty.
- 6. The decrease in the 95 percent confidence range, based on Equation (5), due to project performance. Specifically, the upper end of this range, from  $\overline{H}$  to  $\overline{H}U$  is processed.
  - 7. The project cost.
- 8. The ratio of item (6) divided by item (7). This is the objective factor for the proposed research project in terms of one variable. As indicated, a project may impact on several variables.

The Log-Normal Hazard Assumption. As an example for consideration, the 300 values of current situation hazard of the CFS effect from "condensate water" are used. Some of the characteristics of this sample population are:

Mean = 2118

Uncertainty = \* 20.55

Highest sample value = 111,601 (52.7 x mean)

Lowest sample value = 28 (mean/75.6)

Median = 2017.5

The test performed to assess the distribution is the "goodness of fit" test found in most statistical textbooks such as by Dixon and Massey. The distribution is divided into several intervals and the number of samples that are in each interval is compared to the expected number. For convenience, 10 intervals were used, each expected to include no percent of the samples. The analysis yielded a  $\chi^2$  statistic of 8.53, which is slightly less than  $\chi^2$  (P = 0.75) of 9.04 for 7 degrees of freedom. Informally stated, if the log-normal distribution assumption was rejected, there is somewhat more than a 25 percent chance of being wrong. Statistical evidence to reject the assumed distribution is considered weak.

This exercise is reassuring, since if hazard has the log-normal distribution, uncertainty has the attributes that makes Equation (5) a reasonable statement. From a conceptual outlook, this is essential to the methodology.

The hazards presented in Figure 9 are estimates of mean hazards of log-normal distribution. The means are not known; however, inferences can be made as to how close the estimates are to it. The relation involved is Chebyshev's Inequality, which for the variable used here is written:

Prob (Log 
$$\overline{H}$$
 - Log  $H_{\text{mean}} \le \frac{k \text{ Log } \sqrt{U}}{\sqrt{N}}$ )  $\ge 1 - 1/k^2$  (13)

N is the number of samples used to derive  $\overline{H}$  and k is a factor arbitrarily chosen. For example, if the  $\overline{H}$  above is desired to be within 10 percent of  $\overline{H}_{mean}$ , the probability of this is more than 0.15. For agreement within 20 percent, the probability increases to more than 0.73.

From Equation (13), the hazard computed for the post-research situation is a better estimator of the mean hazard. This hazard can be compared to the deterministic hazard to see approximately how well the two procedures agree. This is done in Table 10 for two effects. There is a general trend for the stochastic computation to generate higher hazards than the deterministic computation. This is expected, as each stochastically-computed hazard is the sum of several individual hazards. Fortuitously, these are so distributed that the sums are reasonably represented by a log-normal hazard.

From the viewpoint of general HRAM applications, this poses a problem. Conceptually, projects with hazards corresponding to Equation (4) could be processed. However, these hazards involve additional summations. Theory predicts a wider divergence between stochastic and deterministic results. This is observed as shown below:

Compound	Total Hazard,  Table 6	Stochastic Total Hazard
"Condensate water"	2342	4223
2,4,6-Trinitrotoluene	3027	6056
2,3,6-Trinitrotoluene	778	1 051
2,4-Dinitrotoluene	516	473
1,3-Dinitrobenzene	496	1102
5-Amino-2,4-dinitrotoluene	488	697
3,4-Dinitrotoluene	190	305
1,3,5-Trinitrobenzene	1 44	287
2,3-Dinitrotoluene	126	211
2,6-Dinitrotoluene	103	1 57

The results in column 3 are included with the run print-out. Hazards from both procedures differ by as much as a factor of two. This may indicate that hazards corresponding to Equation (4) are not well-suited to a

log-normal distribution. This could cast doubt on the validity of Equation (12) as an objective factor when comparisons are made to other projects.

TABLE 10. COMPARISON OF HAZARDS: DETERMINISTIC VS. STOCHASTIC

Effect	Compound	Deterministic Hazard, Table 6	Stochastic Hazard, Figure 9
CFSa	"Condensate water"	1629	2033
CFS	2,4,6-Trinitrotoluene	1749	2287
CFS	2,3,6-Trinitrotoluene	575	596
CFS	2,4-Dinitrotoluene	249	287
CFS	1,3-Dinitrobenzene	307	395
CFS	5-Amino-2,4-dinitrotoluene	350	319
CFS	3,4-Dinitrotoluene	1 39	167
CFS	1,3,5-Trinitrobenzene	85	110
CFS	2,3-Dinitrotoluene	92	112
CFS	2,6-Dinitrotoluene	70	81
С	"Condensate water"	153	178
C	2,4,6-Trinitrotoluene	594	609
C	2,3,6-Trinitrotoluene	12	10
C	1,3-Dinitrobenzene	82	102
C	5-Amino-2,4-dinitrotoluene	19	28
C	3,4-Dinitrotoluene	5	5
00000000	1,3,5-Trinitrobenzene	19 5 31	36
C	2,3-Dinitrotoluene	<b>4</b> 8	5 8
C	2,6-Dinitrotoluene	8	8

Note: All hazards rounded to the nearest integer.

Uncertainty Contributions of Variables to Hazard Uncertainty.
Results from Figure 9 can be used for an analysis of which uncertainties influence the hazard uncertainty. To do this, Equation (3) is rewritten as:

$$H = S \Sigma C*SMB*V*N = S * X$$
populations
(14)

a. Table 6 has the summed hazards of CFS and FKL. From Equations (7) and (8), three-fourths of these hazards are due to the CFS effect.

S is defined as log-normally distributed. There is confidence that H is log-normally distributed. Then "X" should be log-normally distributed. The following is an approximation from which  $U_{\chi}$ , which represents the uncertainty contribution from all other variables, can be estimated.

$$U_{H} = \exp \left[ (\ln U_{s})^{2} + (\ln U_{x})^{2} \right]$$
 (15)

From Equation (15) and appropriate average values of  $\mathbf{U}_{\mathbf{S}}$ , the following  $\mathbf{U}_{\mathbf{S}}$  are determined:

Variable	Current U <sub>s</sub>	Si	tuation U <sub>x</sub>	Post-R	ese U <sub>s</sub>	arc	h Situation
S(CFS)	* 15	*	4.5	*	7	*	4.5
S(FKL)	* 4	*	5.2	*	2	*	5.1
S(C)	* 20	*	6.7	*	7	*	7.0
S(CTR)	*300	*	5.5	*	3	*	7.6
S(CTG)	*300	*	5.4	*	7	*	6.3

These results appear to indicate that in the current situation, with the exception of S(FKL), toxicological factors dominate  $\mathbf{U}_{\mu}$ . After research, non-toxicological factors are of equal or greater effect. A tentative conclusion, based on the comparisons of individual  $\mathbf{U}_{\mu}$ , is that the effect of discharge rate uncertainty predominates over other non-toxicological variables.

An interesting observation is that the  $U_{\chi}$  for human effects tends to be higher than for fish effects. This is probably caused by the uncertainties associated with fish populations (\* 2.3) and with R (\* 3.2). Human populations, on the other hand, have much lower uncertainties, while fish hazards are computed with an exact default R = 1.

Another observation that can be derived from Equation (15) are the uncertainties that would exist at the completion of the most advanced research projects. For humans, "LTM" is generally the most advanced project, although epidemiology may have potential to refine hazard uncertainties.† For fish, a more advanced project exists, that of a

<sup>&</sup>lt;sup>†</sup> From a real-world standpoint, this may be impractical. Ammunition plant production levels vary widely over a period of time, based on the level of military activity of the nation. Thus, real-world exposures over a long period of time would be difficult to correlate with an observable change in the population.

chronic aquatic toxicity test. The S(CFS) uncertainty after such a project is estimated at " \* 2." From Equation (15), the  $\rm U_H$  after such a project† would be about " \* 5.2."

## Objective Factors and Their Interpretation

Since each project involves more than one variable, the relevant ratios are summed to provide an overall objective factor. The overall factor is used to rate the proposed research in comparison to factors of other projects. The factors for the projects, determined after 300 Monte-Carlo simulations, appear in Table 11. The most striking feature of this table is the higher ratings that would be given to "AAT" projects over all "LTM" projects. The cost difference between the two projects is a major cause of these ratings.

Table 11 also includes objective factors that would have prevailed if the analysis had been terminated with a smaller number of simulations. The general trend of the results is established rather early. After the 100th simulation, the factor changes become much less marked. Rating transpositions are restricted to closely-valued projects.

An important question is how precise are the objective factors. At the beginning of this section, it was stated that allocation results are expected to be ordered closely to those of hazard results. Table l1 is so ordered; there is not perfect agreement. The worst situation is that of project "AAT" for 5-amino-2,4-dinitrotoluene. Figure 9 suggests this is caused by the relatively low-sided stochastic hazard computation for the CFS effect, and the relatively small difference between its current and post-research uncertainties. The juxtapositions with "LTM" projects are a function of S(C) as compared with the other human effect dose-risk slopes. If S(C) is relatively low, the contribution of other effects to Equation (12) become more important. This is an example of how uncertainty assignments can influence these factors. This influence is not apparent from hazard valuations.

Each objective factor in Table 11 is a sample taken from a probability distribution of Equation (12). This distribution is defined as a function of sample size. If the characteristics of this distribution were known, statements such as embodied in Equation (13) could be made. Since a variance estimate of the uncertainty is not available, this is not the case.

<sup>&</sup>lt;sup>†</sup> Hazard is assumed to remain constant as a result of such research. This is the most valid conclusion that can be made in the absence of another indication.

TABLE 11. ALLOCATION OBJECTIVE FACTORS OBTAINED AFTER SELECTED MONTE-CARLO SIMULATIONS

			Obje	Objective Factors	Ş	
Project	Compound	300	200	00 L	40	20
AAT	2,4,6-Trinitrotoluene	1223	1310	1183	1468	966
AAT	"Condensate water"	1160	1122	1015	1452	992
AAT	2,3,6-Trinitrotoluene	355	486	515	372	425
AAT	5-Amino-2,4-dinitrotoluene	115	127	123	232	369
AAT	1,3-Dinitrobenzene	225	226	184	127	150
AAT	2,4-Dinitrotoluene	130	116	145	156	229
AAT	3,4-Dinitrotoluene	105	107	129	85	72
AAT	2,3-Dinitrotoluene	72	11	98	104	248
AAT	1,3,5-Trinitrobenzene	65	65	64	141	70
AAT	2,6-Dinitrotoluene	49	45	43	97	165
LTM	2,4,6-Trinitrotoluene	48	39	36	45	129
LTM	"Condensate water"	17	16	18	28	41
LTM	1,3-Dinitrobenzene	9.1	=	14	12	13
LTM	1,3,5-Trinitrobenzene	2.1	2.8	2.7	2.9	2
LTM	5-Amino-2,4-dinitrotoluene	3.4	8	2.7	1.7	3.5
LTM	2,3,6-Trinitrotoluene	0.49	0.72	0.58	0.80	0.42
LTM	2,6-Dinitrotoluene	0.35	0.36	0.54	0.58	0.46
LTM	3,4-Dinitrotoluene	0.52	0.42	0.46	0.40	1.9
LTM	2,3-Dinitrotoluene	0.61	0.75	0.61	0.65	0.89

The most convenient way to evaluate the precision of Equation (12) is by replicated simulations. This provides additional samples of each objective factor. The need to do this will depend upon allocation applications. From a practical viewpoint, it may not be needed for current plans. For future HRAM applications, it is worth developing.

As an example, three additional analyses were performed, each consisting of 100 Monte-Carlo simulations. The overall objective factors from these and the previously discussed analysis appear in Table 12.

The probability distribution of Equation (12) is not known, but probably is somewhere intermediate between a log-normal distribution and a normal distribution. Given the four samples for each factor, assuming a normal distribution is probably reasonable. Statistical procedures allow an estimate of confidence limits for mean overall objective factors to be determined. These limits also appear in Table 12.

With four replications, the ordering of projects is somewhat clearer. The project "AAT" for 1,3-dinitrobenzene is still favored over 5-amino-2,4-dinitrotoluene. The ratings for the project for 2,4- and 3,4-dinitrotoluene are probably lower than that for 5-amino-2,4-dinitrotoluene. The rating of project "AAT" for 2,6-dinitrotoluene above "LTM" for TNT is probably valid. The projects as ordered in Table 12 would constitute the recommended ordering for research.

#### CONCLUSIONS AND RECOMMENDATIONS

HRAM gives the decision-maker insights into several aspects of the TNT wastewater compounds that would have been difficult to attain otherwise.

- 1. A numerical rating for the hazard of these compounds which takes into account known or estimated environmental, toxicological, discharge and demographic data. One unusual result of the hazard computations is that the largest hazard was from TNT in non-"condensate water" situations. Without taking this into account, TNT would have been a compound of intermediate concern as a "condensate water" constituent.
- 2. A numerical rating system of hazard that allows for a comparison between different population types. In the analysis, much of the hazard was fish-oriented. For human hazards, the mutagenic or carcinogenic effect predominated. This predomination is not considered conclusive at this stage of data development.
- 3. A research project rating system based on a plausible economic approach. In the exercise, the research project "AAT" for all nine components considered would have been favored over any "LTM" project. The

TABLE 12. ALLOCATION OBJECTIVE FACTORS AND ESTIMATE OF 90 PERCENT CONFIDENCE INTERVAL OF MEAN FROM FOUR 100 MONTE-CARLO SIMULATION RUNS

		0	Objective Factors	-actors		90% Conf	90% Confidence Interval	terval
Project	Compound	-	2	3	4	Low Limit	Low Limit-Mean-High Limit	h Limit
AAT	2,4,6-Trinitrotoluene	1183	1794	2029	2115	1435	1 780	2125
AAT	"Condensate water"	1015	939	1607	1233	953	1198	1444
AAT	2,3,6-Trini trotoluene	515	685	464	405	418	517	919
AAT	1,3-Dinitrobenzene	184	151	183	473	123	248	372
AAT	5-Amino-2,4-dinitrotoluene	123	191	252	150	126	171	217
AAT	2,4-Dinitrotoluene	145	158	137	164	139	150	191
AAT	3,4-Dinitrotoluene	129	154	120	42	72	111	151
AAT	2,3-Dinitrotoluene	98	109	82	9/	9/	88	100
AAT	1,3,5-Trinitrotoluene	64	103	24	99	55	72	89
AAT	2,6-Dinitrotoluene	43	09	74	38	40	54	29
LTM	2,4,6-Trinitrotoluene	36	33	40	39	34	37	40
LTM	"Condensate water"	18	16	15	8.7	=	14	18
LTM	1,3-Dinitrobenzene	14	8.4	12	16	10	13	15
LTM	5-Amino-2,4-dinitrotoluene	2.7	4.4	3.5	2.5	5.6	3.3	4
LTM	1,3,5-Trinitrobenzene	2.7	1.5	1.8	1.8	1.5	1.9	2.4
LTM	2,3,6-Trinitrotoluene	0.58	0.46	1.7	0.23	0.21	0.74	1.3
LTM	3,4-Dinitrotoluene	0.46	1.3	0.72	0.22	0.29	0.68	-:
LTM	2,6-Dinitrotoluene	0.54	0.42	-:	0.49	0.38	0.64	0.89
LTM	2,3-Dinitrotoluene	0.61	0.22	0.49	0.51	0.32	0.46	0.59

rating system was demonstrated under different levels of Monte-Carlo simulations for a given run and for replicate runs for a given number of Monte-Carlo simulations. For more accurate ratings, the second procedure is recommended.

Many of the data manipulations employed to develop the data base are highly empirical. Since HRAM is a unique approach to the allocation-decision problem, some may remain empirical. Major emphasis has been on consistent methods to process information. This has included:

- a. The processing of concentration data from "condensate water" sample analysis to provide estimates of Q.
- b. The processing of vaporization and photolysis data to provide estimates of LMD.
- c. The processing of mutagenic bioassay data to provide estimates of S(C).

There is a need to improve these methods.

The computations to determine discharge rates point up the danger of non-critical acceptance of concentration data. The decision-maker should be aware of data-processing procedures used in this exercise. Some of the compounds whose presence in wastewater can be masked in the performance of a gas chromatogram are prime candidates for continued studies. Less empirical methods of assessing concentrations derived under such situations should be developed.

The environmental fate of compounds was of great interest to the conferees at the 23-24 February 1978 meeting. In this analysis, the populations at risk were so spaced in travel time that barring gross misassignments of LMD, the sensitivity of results to LMD were not large.

However, several other mechanisms that occur in the environment, such as biodegradation, adsorption in the sediment and reactions with water, have not been included. Even a rough understanding of these mechanisms, given the diversity of the locations and of the real environment, would be a formidable task. Perhaps a standardized set of fate tests may be a more useful approach to providing data for LMD estimates.

Human effects data processing is an area for improvement. The use of potency factors in this study (see page 39) as a scale factor for S(C) is highly speculative. However, as more data are collected by microbial mutagenic bioassay and mammalian carcinogenic and mutagenic bioassay for compounds, such an approach may gain acceptance.

One observation of hazards (Table 7) was that when default S(CTR) and S(CTG) were assigned, the contributions of these effects were small compared to that from S(C). A restudy of the default value assignment procedures may be merited. Another problem is that, within reasonable limits, there will be dose levels at which a compound causes a CTR and a CTG effect. This is not true for a C effect. This conceptual difference is not yet resolved in mathematical terms amenable to HRAM algorithms.

There will be a continuing need to incorporate new information within the HRAM data format. As one example, after the analysis was completed, octanol-water partition coefficient data became available. This may influence LMD, as it may be an indicator of the ability of a compound to adsorb on sediment. It may also influence R for humans, as a larger amount of compound in sediment would be more liable to removal in water treatment processes. It may even cause non-default R to be refined for fish, which would be indicative of different potentials for compound ingestion by fish.

The TNT wastewater study involved compounds with common discharge points and common uncertainty assignments to many data inputs. This allows for in-depth assessment of allocation results. This will not be true in the general case. Because of statistical treatment of data inputs and uncertainties and stochastic methods, the results incorporate certain unusual features. These features are unavoidable.

First, the assumption of log-normal hazard for projects which involve hazards corresponding to Equation (3) was reasonable. This was in part due to a judicious choice of uncertainties for input data variables. Hazards computed as part of the allocation methodology will not be equal to those computed as part of hazard evaluation. They will tend to be higher. For toxicological studies, which are the major projects of concern for this exercise, Equation (3) is applicable. Conceptually, HRAM should be able to assess projects that involve more general hazards, such as that of a compound for all effects, one effect for all compounds, or one location for all compounds. Realistically, the hazards so computed may not be log-normal. This would cast doubt as to whether the allocation methodology would provide valid results according to the objective factor concept.

Rating of research projects involves the summation of two or more objective factors, since the projects effect the uncertainties of more than one effect. This leads to a numerical valuation which is a function of the random number generation sequence and the number of Monte-Carlo simulations. If one simulation set is used, there may be transpositions in ratings due to statistical variance of factors. For a highly discriminating allocation, several simulation runs are suggested. The size of these runs will be a function of the accuracy desired in the analysis and of computer time costs. Fortunately, such costs at this laboratory are low.

For a "rough look" as to how a group of projects may be allocated, one run with 100-300 Monte-Carlo simulations may suffice. The study showed the effect of a more discriminating approach with four replicates of 100 Monte-Carlo simulations. The potential for one or two position transpositions of ratings from what they should be still exists.

Any user should be aware that HRAM results and recommendations ultimately are based on data inputs and algorithms. There is no objective yardstick upon which the validity of HRAM results rests; this is a common trait of rating systems. HRAM is most dependent upon uncertainty assignments. They were, for the most part, arrived at on the basis of consensus. The allocation has a high degree of subjectivity associated with it. The user should avoid being too entranced at the numbers just because they come from a computer. However, critical reviews and refinements based on experiences with HRAM will enhance the confidence with which HRAM is used. This exercise marks a step in this process.

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#### APPENDIX A

#### THE ECONOMIC BASIS FOR HRAM

The adoption of a standard for pollution discharges by a regulator involves the trade-off between two costs: a socioeconomic adverse cost of the pollutant and the cost of abatement. An ideal situation is shown in Figure A-1 for one compound discharge at one location. Both cost functions are well-known; AOB is the socioeconomic cost function and XOY is the abatement cost function. An ideal trade-off (minimize total cost) would cause a standard of  $\mathbb{Q}_0$  to be set. Both costs are  $\mathbb{C}_0$ .

In reality, the abatement cost function may be fairly well known, but the socioeconomic function is not. Since a regulator bears a public responsibility to provide ample margins of protection, the regulator perceives a function skewed above the socioeconomic cost. As shown in Figure A-2, this curve is RST. The regulator wishes to maintain a socioeconomic cost of  $\mathbf{C}_{\mathbf{0}}$ . To do so with the perceived function RST requires a standard of  $\mathbf{Q}_{\mathbf{Set}}$ . This required additional abatement at an additional cost of  $\mathbf{C}_{\mathbf{Set}}$ - $\mathbf{C}_{\mathbf{0}}$ .

In HRAM context, Equation (4) represents a point of AOB. Given different levels of Q, a complete curve could be generated. In HRAM context, RST represents the product HU as a function of Q. Of interest is the point S and the perceived cost  $C_{\rm S}$ . S is indicative of some operating capacity, such as full capacity.

The plant operator may accept the existing situation and proceed to spend  $C_{\text{set}}$  for abatement. As an alternative, he can convince the regulator that research will decrease the uncertainty of the perceived social-cost function. After such research, the situation of Figure A-3 occurs. The perceived function is R'S'T'. Using the same approach as before, the standard can now be increased to  $Q'_{\text{set}}$ . The corresponding abatement cost is  $C'_{\text{set}}$ .  $C'_{\text{set}}$  has been saved.

Prior to this research, the perceived socioeconomic cost of current discharges was  $C_s$ . After research, it is  $C_s'$ . For a given amount of abatement savings, it can be seen that the optimal research project is that which maximizes  $[(C_s - C_s')/\text{research cost}]$ . This can be recognized as the objective factor of HRAM.

But the HRAM problem is often the obverse; to show that a given objective factor maximizes the abatement savings. This can be proven given that XOY is either linear or concave upwards. This is not a stringent limitation.

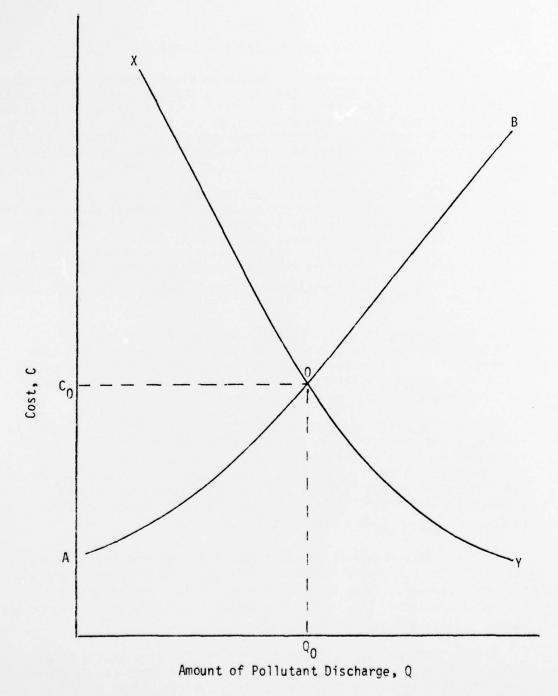


Figure A-1. The Ideal Trade-Off of Socioeconomic and Abatement Costs.

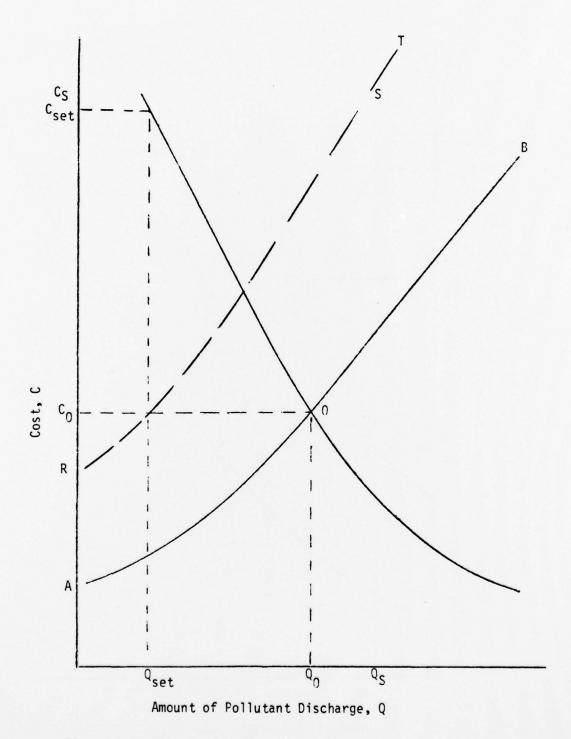
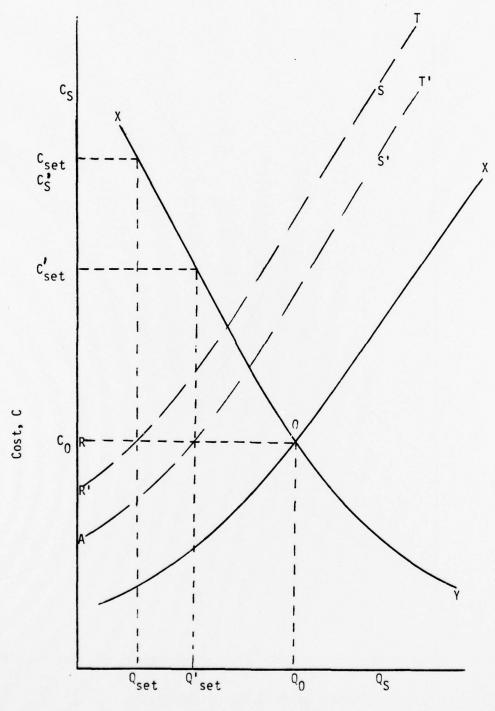


Figure A-2. The Trade-Off Under Conditions of an Uncertain Socioeconomic Cost Function.



Amount of Pollutant Discharge, Q

Figure A-3. The Trade-Off Under Condition of a More Certain Socioeconomic Cost Function.

Research may also cause a shift in AOB in that not only does a decrease in uncertainty occur, but so does the refinement of one or more components of hazard. Since these are not a priori known (if they were, the function would have been a priori adjusted), AOB must be assumed constant for the pre- and post-research analysis.

## ACRONYMS AND SYMBOLS USED IN THIS REPORT

NOTE: Several subscripts identified in Table 1 and Figure 1 are not cited here.

# ACRONYMS

AAT	Acute aquatic bioassay research project
AHED	Adjusted human equivalent dose
C	Carcinogenic or mutagenic effect in humans
CFS	Chronic toxicity effect to fish
CTG	Severe chronic toxic effect to humans
CTR	Mild chronic toxic effect to humans
48EC50	Concentration to effect 50 percent of population after 48-hours exposure
FKL	Episodic fish kill
FSH	Fish population identifier
H20	Surface water transport medium identifier
HRAM	Hazard Ranking and Allocation Methodology
HUM	Human population identifier
96L 50	Concentration lethal to 50 percent of population after 96-hours exposure
LTM	Lifetime mammalian feeding research project
PRO	Research project identifier
RDX	Cyclotrimethylenetrinitramine
TNT	2,4,6-Trinitrotoluene
	SYMBOLS OF VARIABLES
С	Concentration (mg/liter) in body of report. In Appendix, a cost
Н	Hazard (\$/year); H, estimate of mean hazard; H <sub>mean</sub> , mean hazard
LMD	Environmental disappearance rate constant (year <sup>-1</sup> )
N	Population identifier. In Equation (13), number of simulations.
Q	Discharge rate of compounds to surface waters (kg/year)
R	Water treatment retention factor

S	Dose-risk slope. For human, units are gram <sup>-1</sup> , for fish, liter/mg-year
SMB	Concentration-dose conversion factor
SMF	Surface water flow (liter/year or ft <sup>3</sup> /sec)
SMT	Travel time (days)
U	Uncertainty. Often subscripted with referred variable
V	Socioeconomic cost (\$/population unit) or an undefined variable (see HRAM As Applied To Surface Water Pollution)
X	Non-toxicological overall variable defined in Equation (14)
h	Sample value of hazard in Equation (5)
k	Constant in Equation (13)
x <sup>2</sup>	Chi-squared statistic

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